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BIOASPEN: SYSTEM FOR TECHNOLOGY DEVELOPMENT

Interim Report

Submitted to

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by

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1. OBJECTIVES AND SCOPE

The objective of this project is to develop a realistic biotechnology assessment tool. Its main benefit is seen as providing ECUT and industrial chemical manufacturers with a consistent basis for examining proposed bioroutes to bulk chemicals. The basis of this tool would be currently available technology but would allow asking 'what if' types of questions and thereby ascertain the total potential impact of new technology were it to be developed in either energy conservation or biochemistry (recombinant DNA related types of technology). During the course of these evaluations, the energy requirement of bioprocesses, including upstream processing (raw material preparation), sterilization, media preparation, fermentor (reactor) requirements, and downstream processing, which includes cell-liquid separations, solute-liquid separations, dryers and packaging and various interactions which can occur when 'what if' types of questions are asked, will become more clearly understood and documented. This will be of value to ECUT in deciding which areas of bioprocess technology would most usefully profit from government-sponsored research and yet constitute too high a risk for industry to sponsor alone.

DOE/ECUT is concerned with bulk commodity applications of bioprocesses. Considerably less emphasis should be placed on bioroutes to new pharmaceuticals and small-scale specialty chemicals whose high value-added market potential more than justifies any unit cost of energy. The project directs computer analysis at large scale processing, where even small but significant savings of energy on a unit basis have a broad impact on the

national energy budget.

What is being offered is an accurate tool for consistent analysis of bioprocesses across a spectrum of potential applications. This assessment can yield precise information about where DOE should encourage new research to provide the nation with large scale renewable raw material resources and energy-conservative technology. It opens up a gauge of prospective success for any high technology group wishing to evaluate the results of genetic engineering research.

Industry is too constrained by short-range concerns to undertake the long-range research which will bring the potential of bioprocessing of renewable resources to fruition. Witness the recent abandonment of major synfuels projects by industry when the price of petroleum stabilized. Nevertheless, it is in the national interest that replacement technology be available 10 or 20 years from now. Non-renewable raw materials will dry up inevitably. The potential of bioprocessing to make even non-renewable materials more attractive than conventional processing in the long run is not discounted.

The System for Biotechnology Assessment is a small investment in the future. The cost is greatly transcended by its promise of rapidly screening opportunities and goals for DOE/ECUT. This tool would also serve as a valuable training and screening facility both in academia and industry.

The specific objective is to convert the existing computer program known as DOE-ASPEN to function for bioprocesses. ASPEN was developed successfully to allow assessment of synfuel projects. The changes would add the unit operations peculiar to

bioprocesses and bioseparations, such as fermentation. The data base would be extended to include bacterial and cell properties. The costing routines would be updated and extended. To validate the system the already documented acetone-butanol process would be examined, as well as selected other bioprocesses of interest to ECUT/DOE. It is anticipated that towards the middle of the project a consortium of industrial companies would be formed to continue and refine the development of this tool and to facilitate its transfer to industry. This group should include representatives of both large and small firms.

A second, and unfunded, phase of the project is contemplated to begin in the later stages of the work. This would analyze the potential of developing a single technology assessment tool that can be executed on a user-friendly microcomputer such as an IBM Personal Computer. The downsizing of the large model would have to be done with some attention to the level of confidence attainable with restricted models.

2. INTRODUCTION

The chemical and petroleum processing industry is faced with increasing shortage of raw material and increased costs of production over the next two decades. As petroleum supplies dwindle it will be more and more dependent on renewable resources. The new processes, based on biocatalyzed conversions, hold a high potential of providing an alternative source of raw material and energy for the U.S. chemical industry. Although these processes are not currently competitive with other conventional sources, further research into new catalysts, new routes and improved engineering (reactors and separation processes) for production are increasing their potential.

The question naturally arises as to what processes hold the greatest potential and what areas are most critical in terms of research needs. One would like to concentrate available resources on those concepts which hold the greatest opportunity for improved efficiency and production of alternative fuels for use in energy conversion systems.

At present no form of computer-based bioprocess analysis system exists. There is a need for such a system for the following reasons:

- (1) Bioprocesses are currently perceived as a major opportunity in the chemical and process industries
- (2) Different groups of investigators arrive at different assessments of whether a particular process is economic or not
- (3) Such assessments of bioprocesses are of necessity limited and use different starting assumptions
- (4) DOE/ECUT is faced with information of this type and has few

methods of assessing its worth. It then has to decide which, if any, biotransformations are worth supporting. In particular, it must attempt to identify the weak links within a process, strengthening of which would allow the process to succeed.

A TOOL FOR TECHNOLOGY ASSESSMENT is needed rather than a plant design tool. However, the degree of detail needed in process analysis for a realistic estimate of the worth of a bio-process is considerable. Part of the problem with the type of analysis available from consulting firms is that it inevitably can only provide answers to within 30-50% accuracy. This degree of doubt is rarely, if ever, made explicit. It is not surprising that industry, knowing these limitations, will be slow to move even on an optimistic forecast. However, recognition of, for example, the advantages of a 2-5% improvement in yield could in many cases be sufficient to persuade a bulk producer to switch to a bioroute for a desired product. The producer therefore needs a sufficiently accurate analysis to enable him to make that decision.

It is anticipated that the models developed will have high comparative accuracy and a high degree of uniformity. They will allow, 1) direct comparison with conventional routes to the same chemicals, and 2) ranking of a range of proposed bioprocesses in order of likely economic return. This will permit ECUT to identify research needs and targets more closely. Absolute accuracy in such models is less necessary and will depend largely on the detail of the simulation.

(5) The system will allow individual companies to ask 'should chemical A be made by a biological route?'. The answer will

depend on who is asking the question, when, and for which location. Each company has its own specific special circumstances that it is usually unwilling to discuss publicly. These may include special feedstock agreements at favorable prices, convenient access to markets or raw material sources: a company may already have byproducts available from one plant that can be utilized in another, or special interest rates and risk factors. Furthermore each variable will be subject to change as the company grows or diversifies and as the external environment changes, e.g. oil prices, and as management attitude to perceived risk changes.

None of the above factors can be influenced directly by ECUT. They can be turned to advantage by providing a technology assessment tool that allows the question to be investigated directly by the end user, with explicit regard to his particular circumstances, but without either the circumstances or the answer being disclosed to outside parties.

(6) Much of the technical thrust for the development of biotechnology has come from small companies consisting of outstanding molecular biologists, etc. Their main interests do not and, at least for now, cannot be in the development of sophisticated economic and technology assessment tools. The proposed technology assessment tool would permit them to identify and exploit relevant research and commercial goals.

Despite the requirements of a mainframe computer, the program would be directly available through timesharing systems over the telephone lines, and hence directly available to smaller companies.

(7) The development of the technology assessment programs would

constitute valuable training for the graduate students concerned. After graduation they would be well placed to transfer this training to an appropriate biotechnology-based industry. The availability of the programs would also offer many institutions the opportunity to enhance their educational and training activities in this most valuable component of the nation's future economic well-being.

3. SUMMARY OF TECHNICAL PROGRESS

The public version of ASPEN available through the Argonne National Energy software center was installed in the Chemical Engineering Department VAX 11/750 computer. To examine the idea of BIOASPEN, a test example (the manufacture of acetone, butanol and ethanol through a biological route) was chosen for simulation. Previous reports (1, 2) on the BIOASPEN project have shown the limitations of ASPEN in modeling this process.

To overcome some of the difficulties, modules were written for the acid and enzyme hydrolyzers, the fermentor, and a sterilizer. Information required for these modules was obtained from the literature whenever available. Additional support modules necessary for interfacing with ASPEN were also written. Some of the ASPEN subroutines were themselves altered in order to ensure the correct running of the simulation program. After testing of these additions and changes was completed, the Acetone-Butanol-Ethanol (ABE) Process was simulated.

A new release of ASPEN (which contained the Economic Subsystem) was obtained and installed. This subsection was tested, and numerous changes were made in the FORTRAN code. Capital investment and operating cost studies were performed on the ABE Process. Some alternatives in certain steps of the ABE simulation were investigated in order to elucidate their effects on the overall economics of the process.

4. DETAILED DESCRIPTION OF TECHNICAL PROGRESS

This section describes in detail the progress made in the various aspects of the project to date.

4.1 Installation of ASPEN

The public version of ASPEN was installed in the Chemical Engineering VAX computer. The test examples provided by the Morgantown Energy Center were run through the program. UOSD, the test problem for the solids handling modules, could not be run because of the lack of sufficient documentation. Work was therefore started on the development of a documentation aid for ASPEN programmers, which would give information on the hierarchy of subroutines used in any process module. With the installation of the later version of ASPEN (version 6), this work was discontinued as an on-line documentation aid had been provided with the package.

4.2 Incorporation of New Models into ASPEN

ASPEN, as is, was considered inadequate to model various aspects of the ABE Process (1, 2). It was considered essential to model the acid and enzyme hydrolyzers, and the fermenter. A sterilizer was also incorporated into ASPEN. While the actual FORTRAN code for each of the modules may be found in the Appendix, this subsection provides information on the actual models used in each of these units.

(i) Acid Hydrolysis:

The kinetic model in general use (3, 4, 5, 6 etc.) for the cellulose hydrolysis seems to be the model proposed by Saeman (7):

crystalline cellulose ---> glucose ---> degradation products

amorphous cellulose ---> glucose ---> degradation products

Chambers (8) proposed a similar model for hemicellulose hydrolysis:

hemicellulose ---> xylose ---> degradation products

The rate constants k_i , follow the Arrhenius rate form:

$$k_i = A_i \exp(-E_i/RT)$$

with the pre-exponential factor A_i being a function of acid concentration as follows:

$$A_i = A_{oi} C^m$$

The kinetic constants used in this work were reported by Bhandari et al (6). They make the assumption that the amorphous cellulose, which is the easiest fraction of cellulose to hydrolyze, is attacked and converted instantaneously to glucose. Therefore, an initial yield of glucose was assumed equal to the amount produced from the amorphous cellulose. They made a number of experimental runs, and produced best-fit equations for cellulose and hemicellulose hydrolysis reaction constants based on corn stover as substrate:

$$k_1 = 2.7 \cdot 10^{19} C^{2.74} \exp(-45,300/RT)$$

$$k_2 = 2.01 \cdot 10^{14} C^{1.86} \exp(-32,800/RT)$$

$$k_3 = (7.64 - 3.68/C) \cdot 10^{20} \exp(-41,000/RT)$$

$$k_4 = (4.60 - 1.95/C) \cdot 10^{14} \exp(-32,000/RT)$$

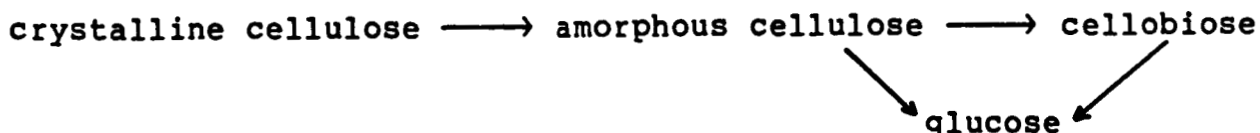
They also present a table comparing their kinetic constants with those available in the literature for other substrates. Some of this data along with kinetic constants presented by Kwarteng (5) for Aspen wood are shown in Table 4.1, and are incorporated into the user model.

(ii) Enzyme Hydrolysis:

The literature provides a number of models that may be used for the enzymatic hydrolysis of cellulose (9, 10, 11, 12 etc.). Most of them however, are applicable to restricted systems (specified substrates and microorganisms), or require enormous numbers of parameters to be specified. In order to keep the model simple at this time, it was decided to use rate expressions presented by Pietersen et al (12). This model does make a large number of assumptions, but also contains elements of the common observables of enzymatic hydrolysis of cellulosic substrates:

- (1) Cellulose consists of a crystalline and an amorphous region.
- (2) Michaelis-Menten kinetics may be used.
- (3) Reactions are subject to product inhibition.
- (4) The organism grows on glucose, with a Monod growth rate.

The reaction scheme is as follows:



The different rate expressions (in g/liter hr) are:

- 1) crystalline cellulose to amorphous cellulose

$$\text{rate} = 0.959 \left[\frac{[C] [E]}{2.14 + [C] + \frac{[E]}{46.5[A]}} \right] \text{ g/liter hr}$$

Table 4.1 Comparison of Rate Parameters for Acid Hydrolysis
(Different Substrate Materials)

Substrate Material	Preexp. Factor		Acid Concentration		Activation Energy	
	$\bullet 10^{-10} (\text{min}^{-1})$	$\bullet 10^{-14}$	m_{c1}	m_{c2}	E_{c1} (kcal/gmol)	E_{c3}
Douglas Fir	17.3	2.38	1.34	1.02	42.9	32.87
Kraft Paper	280	4.9	1.78	0.55	45.1	32.8
Solka Floc	12.2	3.79	1.16	0.69	45.2	32.8
Oak Sawdust	4.4	0.028	1.00	1.80	42.9	30.0
Corn Stover	27.1	2.01	2.74	1.86	45.3	32.8
Aspen	1.45D-3	3.84D-5	1.16	0.57	33.7	21.0

ii) amorphous cellulose to cellobiose

$$\text{rate} = 31.3 \left[\frac{[A]^{0.6} [E_c]}{30.4 + [A] + 9.74[B]} \right] \text{ g/liter hr}$$

iii) amorphous cellulose to glucose

$$\text{rate} = 4.12 \left[\frac{[A] [E_c]}{44.1 + [A] + 2.25[G]} \right] \text{ g/liter hr}$$

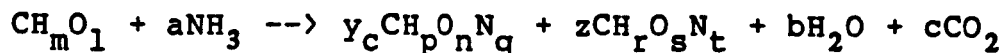
iv) cellobiose to glucose

$$\text{rate} = 3.58 \left[\frac{[B] [E_b]}{0.265 + [B] + 0.376[G]} \right] \text{ g/liter hr}$$

Here, concentrations are in g/liter and the enzyme concentrations $[E_c]$ and $[E_b]$ are in FPU/ml (filter paper units of cellulase activity) and BU/ml (cellobiase units of β -glucosidase activity). The microorganism used in their study was T. Reesei, QM 9414, which is the same as that used in the present model.

(iii) Acetone-Butanol-Ethanol Fermentation:

For an anaerobic fermentation, a balance equation may be written:



The problem however, is in determining the yield coefficients (a, b, c, y_c, z), and the kinetics of the reaction system.

The reaction kinetics and the yield coefficients depend on the biochemical pathways available to the system. For butyric acid bacteria, these pathways for glucose fermentations are numerous (see Figure 4.1) and complex, involving a large number of intermediate/final compounds. Moreover, the kinetics of each step are not known. An analysis of the pathways however, yields impor-

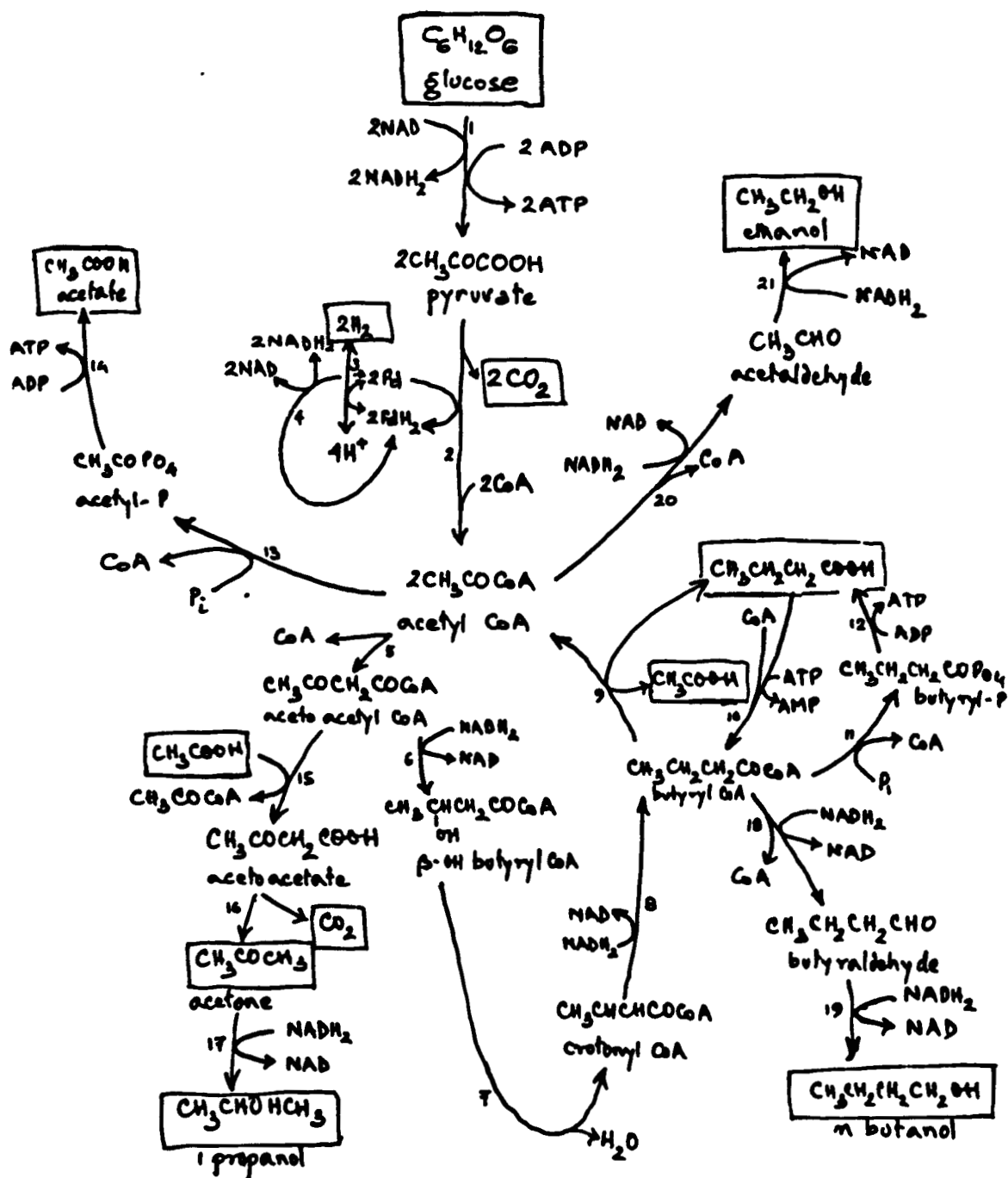
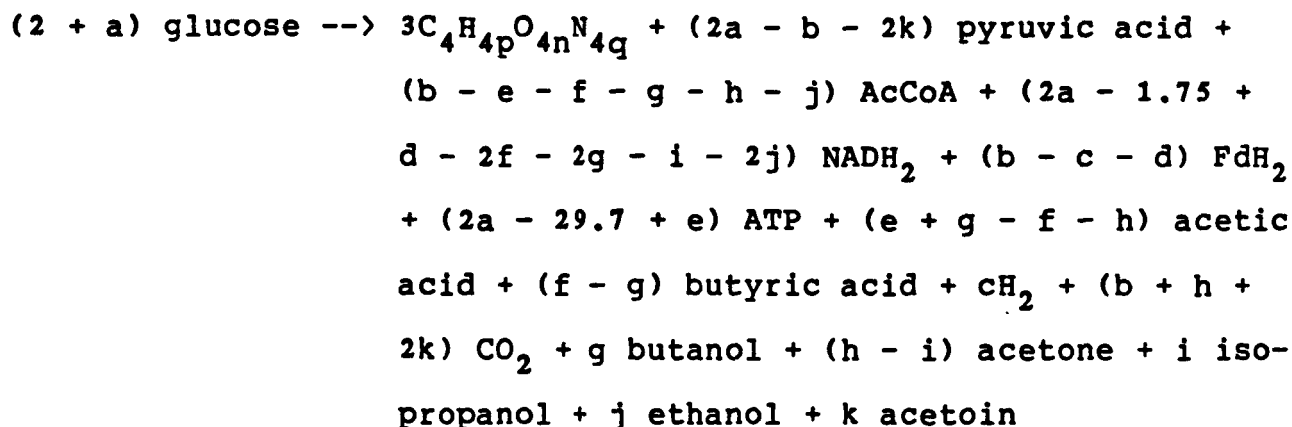


Figure 4.1 Biochemical Pathway of Glucose Fermentation by Butyric Acid Bacteria

tant information on the yield coefficients. This topic has been addressed in detail by Papoutsakis and his coworkers (13, 14), and they present an overall equation for solvent production as follows:



To fully determine the above, the 11 constants a through k have to be determined. Some additional equations are valid for these fermentations, and they are listed below:

$$2a - b - 2k = 0$$

$$b - e - f - g - h - j = 0$$

$$2a - 1.75 + d - 2f - 2g - i - 2j = 0$$

$$b - c - d = 0$$

The above equations are valid because AcCoA, NADH₂, FdH₂ and pyruvic acid do not accumulate in the fermentation broth. These equations have been shown to include the Carbon balance and an available electron balance. Also, the derivation of the overall equation includes the assumption that (i) the ATP yield $Y_{\text{ATP}} = 10.5 \text{ g/mol}$, and (ii) the fraction of carbon in biomass, $\phi = 0.462 + 0.023$. The overall equation has been shown (13), based on data available in the literature, to be valid.

A computer survey of the literature produced only one model for the ABE fermentation (15). The results reported were not

reproducible, possibly because of an error in some parameter. Therefore, in the absence of any kinetic model for the fermentation, a yield-based model utilizing the overall equation was used. For the purposes of BIOASPEN at the present time, kinetics are not as important as the knowledge of correct yield values of the products. This is because the yield coefficients have an immediate effect on the economics of the process. Therefore, a Monod growth model of biomass growth and substrate (glucose) utilization was used, with the product formation being linked directly to growth. It should be noted that this model would therefore not show the production of acids (which are intermediate products in the biochemical pathways) prior to solvent formation.

(iv) Sterilization:

Sterile operation in bioprocessing is critically important and may account for a fair proportion of operating costs. Heat sterilization, whether continuous or batch, is also energy intensive. Extensive discussions on sterilization may be found elsewhere (16). A short description of the model equations for the kinetics of thermal death is presented here.

Logarithmic death rates may be represented by:

$$\frac{N}{N_0} = \exp(-kt)$$

For bacterial spores, the non-logarithmic death rates that are found may be described by a sequence of reactions, in which the formula becomes:

$$\frac{N}{N_0} = \frac{k_r}{k_r - k_s} \left[\exp(k_s t) - \frac{k_s}{k_r} \exp(-k_r t) \right]$$

The rate constants k , k_r and k_s may be represented by the Arrhenius rate forms:

$$k = A \exp\left[-\frac{\Delta E}{RT}\right]$$

Deindorfer and Humphrey (17) describe equations for batch sterilization. The del factor ∇ is defined as:

$$\nabla_{\text{tot}} = \nabla_{\text{heat}} + \nabla_{\text{hold}} + \nabla_{\text{cool}} = \ln \frac{N}{N_0} = A \exp\left[-\frac{\Delta E}{RT}\right] dt$$

The time-temperature relationships for heating and cooling depends on the method of heating/cooling, and are shown in Table 4.2.

Depending on the values of the various parameters (such as heat transfer coefficients, temperature of sterilization, flow rates of steam) the steam requirements may be worked out.

For continuous sterilization, one may use the continuous injection method or the continuous plate exchanger. In both cases, extra units are required in addition to the steam, adding to the capital costs. The material balance may be written as:

$$\frac{d^2N}{dX^2} - Pe \frac{dN}{dX} - PeDaN = 0$$

where $N = N/N_0$

$Pe = \text{Peclet number} = UL/D_z$

$D_z = \text{axial dispersion coefficient}$

$X = X/L$

$Da = \text{Reaction number} = kL/U$

$U = \text{average velocity}$

$L = \text{length of the unit}$

Table 4.2 Temperature-Time Profiles in Batch Sterilization

Type of heat transfer	Temperature-time profile	Parameters
Steam sparging	$T = T_0 \left(1.0 + \frac{at}{1 + bt} \right)$ hyperbolic	$a = \frac{hs}{MT_0 \rho C_p} \quad b = \frac{s}{M}$
Electrical heating	$T = T_0(1.0 + at)$ linear	$a = \frac{q}{MT_0 \rho C_p}$
Steam (heat exchanger)	$T = T_H(1 + be^{-at})$ exponential	$a = \frac{UA}{Mc} \quad b = \frac{T_0 - T_H}{T_H}$
Coolant (heat exchanger)	$T = T_{c0}(1 + be^{-at})$ exponential	$a = \frac{wc'}{M\rho C_p} (1 - e^{-U A / wc'})$ $b = \frac{T_0 - T_{c0}}{T_{c0}}$

where h = enthalpy differences between steam at sparger temperature and raw medium temperature

s = steam mass flow rate

M = initial medium mass

T_0 = initial medium temperature

q = rate of heat transfer, kcal per unit time

U = overall heat-transfer coefficient, kcal/m²·h·°C)

A = heat-transfer area, m²

T_H = temperature of heat source

w = coolant mass flow rate

c' = coolant specific heat

T_{c0} = coolant inlet temperature

ρ = medium density

C_p = medium heat capacity

The boundary conditions are:

$$X \rightarrow 0 \quad \frac{dN}{dX} + Pe(1 - N) = 0$$

$$X \rightarrow 1 \quad \frac{dN}{dX} = 0$$

The solution to the differential equation is:

$$N|_{X=1} = \frac{4y \exp(Pe/2)}{(1+y)^2 \exp\left[\frac{Pe y}{2}\right] - (1-y)^2 \exp\left[-\frac{Pe y}{2}\right]}$$

$$\text{where } y = \left[1 + 4\frac{Da}{Pe}\right]^{0.5}$$

The Peclet numbers may be estimated for fluids flowing in circular pipes at various fluid dynamic conditions. The length requirements may therefore be calculated, or alternatively, with a given length one may calculate $N|_{X=1}$.

4.3 Testing of the Economic Subsection in ASPEN

The new release of ASPEN (version 6) contained the costing modules missing from the previous release. Sample problems were formulated and run on this new system, to verify the smooth running of this subsection. Major problems surfaced during these exercises. These were all corrected, and the changes in the FORTRAN code for each subroutine were listed in a separate sub-directory. The original subroutines were also retained so that a proper account was kept of each change.

4.4 Simulation of the ABE Process

A flowsheet was formulated based on a report by Chem Systems Inc. (18), and ASPEN was used to simulate this. Figure 4.2 shows the broad subsystems in the process. The ABE Process basically

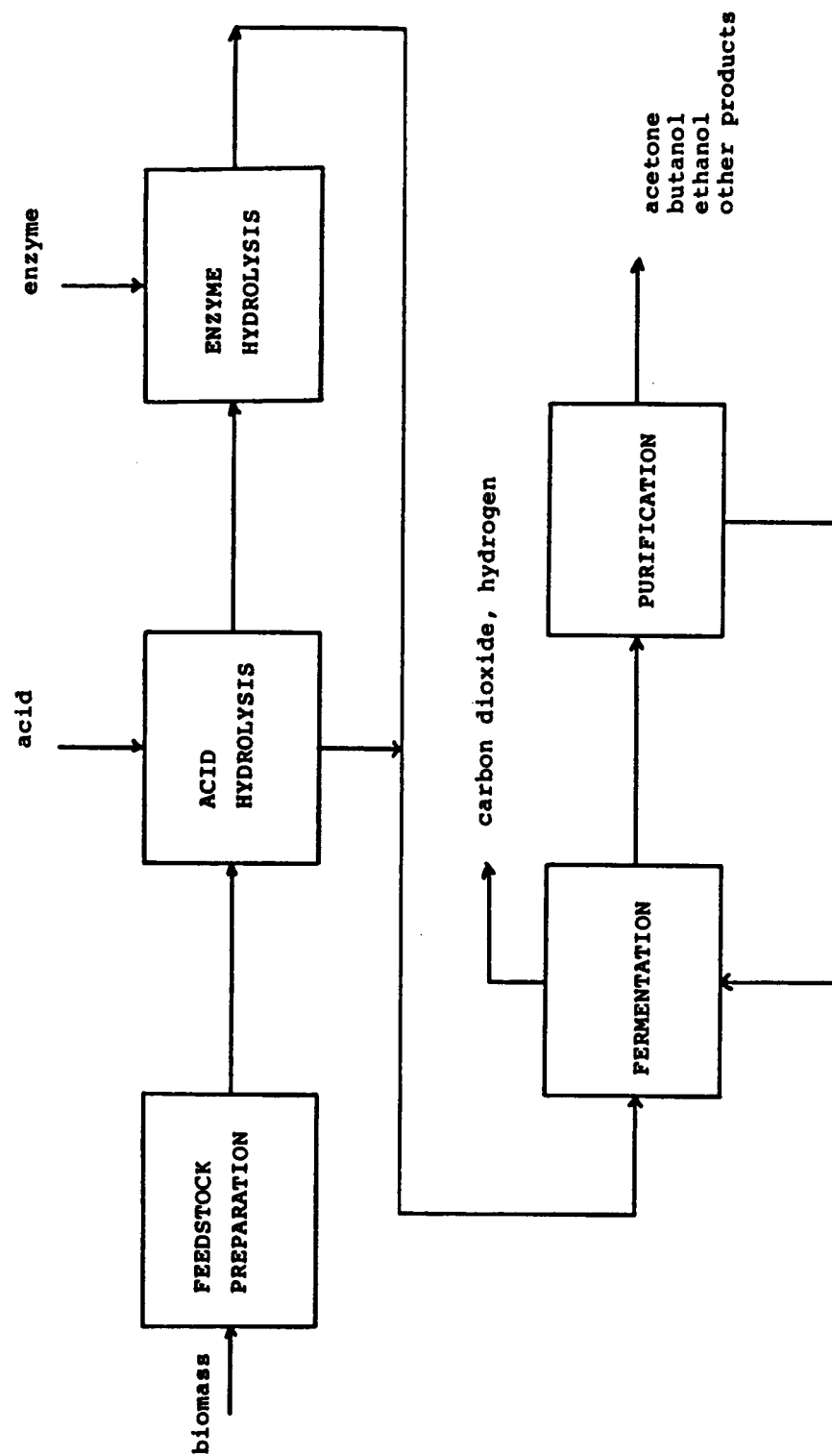


Figure 4.2 Overall A - B - E Process

consists of fermentation of sugars to solvents. A biological route to the formation of sugars from the cellulosic components of wood is also incorporated, resulting in the six-part process described below.

(i) Prehydrolysis

Acid hydrolysis under carefully controlled conditions (0.5 percent H_2SO_4 , 374 deg. F, 185 psia, 12 secs residence time in a plug flow reactor) causes the conversion of hemicelluloses and amorphous celluloses - which are the cellulosic components of wood - to glucose and xylose. Some of the cellulose is converted to the degradation products, hydroxymethyl 1-2-furfuraldehyde and furfural. Wood chips are slurried in a prehydrolysis slurry tank where they are slurried to 35 percent solids, and conveyed to a plug flow reactor. The product stream is immediately quenched, to reduce the degradation reactions. The solids are separated from this stream and sent to the enzyme hydrolysis section, while the soluble sugars are sent to the fermentation section.

(ii) Enzyme Hydrolysis

The remaining unconverted cellulose (crystalline cellulose) is hydrolyzed enzymatically to glucose in this stage. The enzymes are produced by a mutation of T. Reesei, RUT-C-30. Typical conditions required for this stage are 122 deg. F, a pH of 4.8 and hydrolysis time of 24 hours. Conversions of cellulose to glucose may be as high as 90 mol percent, with terminal glucose concentrations of the order of 5 percent.

The solids from pretreatment are slurried and fed to the enzyme hydrolyzers, which are cone-roof atmospheric tanks with heating coils. The product stream is filtered, with the filtrate

going on to fermentation. The solids, consisting mainly of lignin and unconverted cellulose are burnt as fuel.

(iii) Enzyme Production

A mutation of the T. Reesei fungus, RUT-C-30, produces endo-gluconase and β -glucosidase, the enzymes required for enzyme hydrolysis. Continuous fermentation at 86 deg. F and a pH of 4.8 is done with ligno-cellulose as a carbon source and corn-steep liquor as nitrogen source. Other nutrient requirements are provided for by adding organic salts. The outlet from the fermentor is centrifuged: the filtrate is sent to the enzyme hydrolysers, while a portion of the solids is recycled to the fermentor and the remainder is recovered as a single cell protein by-product.

(iv) Fermentation

Fermentation of the sugars is done with *C. acetobutylicum*. Since the microorganism cannot tolerate a butanol concentration greater than 1-3 percent, there is a limit to the initial sugar concentration (6 percent) that may be used. Experiments however, have shown that the yield on this fermentation begins to decrease as the initial sugar concentration is increased beyond 3 percent. Accordingly, the Chem Systems report studied two cases: one maximizing yield, and the other with a 5 percent initial sugar concentration. Since the latter case was shown to be more economical, it was chosen for this study.

A typical yield for this case is 30.6 percent on 90 percent sugar utilization after 48 hours fermentation time. The overall yield is thus 27.54 percent, with a solvent ratio of 61.7 percent butanol, 31.8 percent acetone and 6.5 percent ethanol. Corn is used as a growth medium for *C. acetobutylicum* culture maintenance,

and ammonium sulfate as the nitrogen source. Calcium carbonate and superphosphate are also required in small amounts.

The fermentation vessels are cone-roof tanks in which the sugar streams from prehydrolysis and enzyme hydrolysis, the nutrient media and the seed inoculum are added during the fill period. CO_2 and H_2 evolved during fermentation is sent to the CO_2 recovery section, and the fermentation beer is sent to a beer well prior to purification.

(v) Purification

In this section, the product stream from fermentation is split into pure acetone, butanol and ethanol. A sequence of distillation columns is used for this purpose. Steam costs in this section are extremely high, mainly because the outlet stream from fermentation is very dilute.

(vi) Carbon Dioxide Recovery

Because the amount of carbon dioxide produced during fermentation is large (as much as 3.3 ft^3 per lb of sugar consumed), it is economical to recover this as liquefied CO_2 for sale.

The off-gas is passed through a water scrubber to remove impurities and then compressed. This compressed gas is then passed through activated carbon columns to remove other impurities and is then chilled. The chilled gases then pass to a stripper-condenser system, where the CO_2 is separated from the other gases.

A simulation was carried out using the user modules as described in Section 4.2. Some sample input data files and output reports can be found in the Appendix. The separation of the products from the fermentation broth involves fairly complex distillation column calculations, including azeotropic

calculations . The flowsheet presented by Strobel and Bader (19) uses an improved separation sequence (see Figure 4.3) than that used in the conventional 1950's scheme (here shown in Figure 4.4). In this scheme, the butanol-water azeotrope is separated earlier. A beer column concentrates the broth to near the azeotropic composition and feeds it to a decanter. The butanol-rich phase is fed to a second column, from which a pure butanol stream is withdrawn. The third column does an azeotropic separation, with a butanol-water mixture being recycled back to the decanter. The acetone and ethanol are separated further downstream. The improvements of this process over the conventional one are: (i) the major product, butanol, is removed earlier, resulting in lower flow rates downstream, and (ii) there is one less column required in the overall scheme.

This flowsheet was therefore used for the present simulation. Rigorous calculations however, were not performed for any of the distillation columns; instead, a sequence of splitters and mixers with defined splits (based on the calculations of Strobel and Bader) were used. For the costing exercises, the sizing calculations performed by the same authors were used, as they considered a product stream of a similar flow rate as that produced by the present ABE simulation.

Figures 4.5 through 4.7 show the process flowsheet. Wood chips enter the mill (Figure 4.5), where they are crushed. The crushed wood is slurried in a tank, and then introduced into the acid hydrolyzer at the appropriate conditions. The quench serves to arrest the degradation reactions. After further cooling, the soluble sugars are separated from the crystalline cellulose and

20. beer column 23. butanol/water remover
 21. decanter 24. acetone separator
 22. Butanol stripper

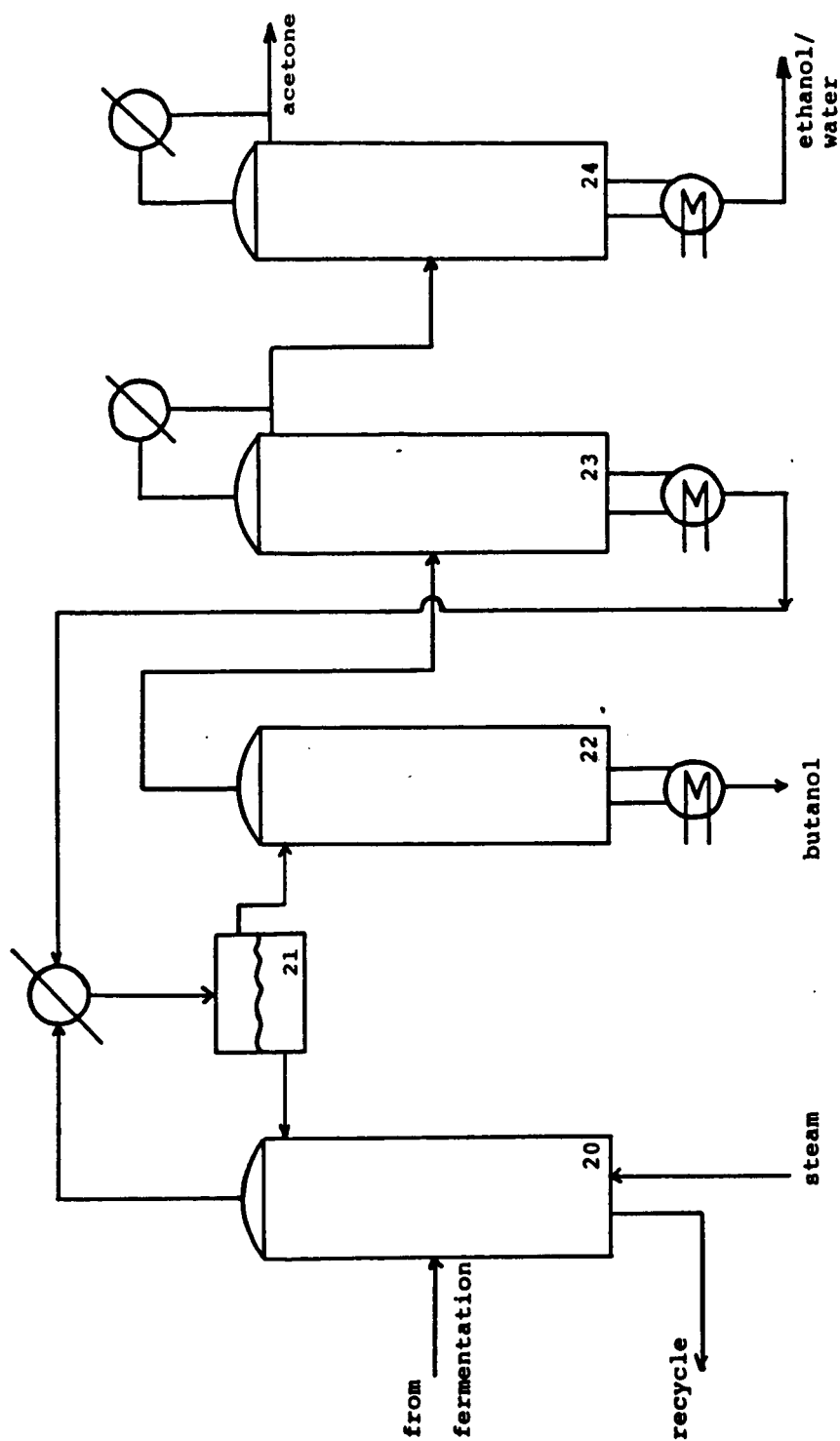


Figure 4.3 Improved Separation Sequence

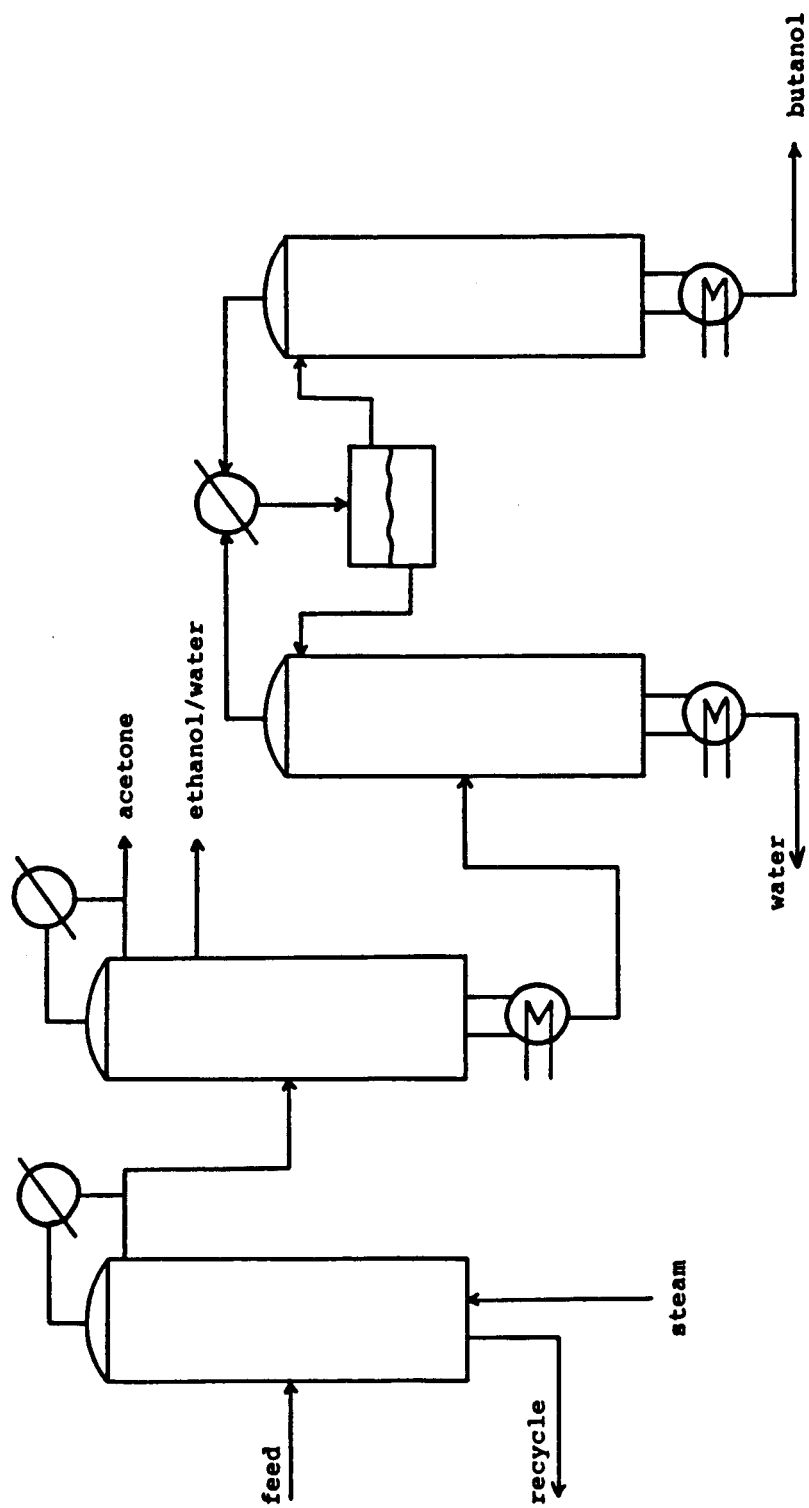


Figure 4.4 Conventional Separation Scheme

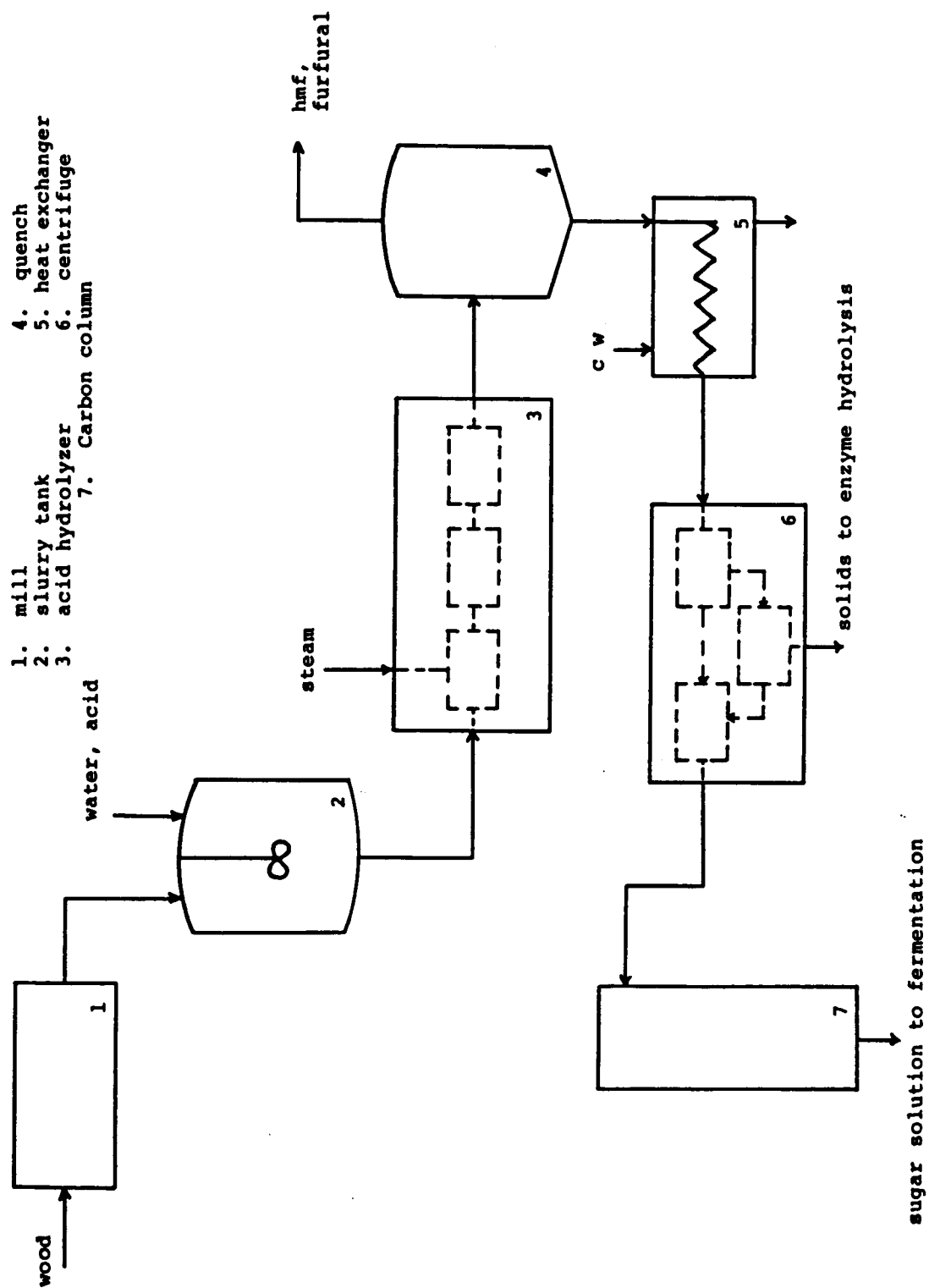


Figure 4.5 Acid Hydrolysis

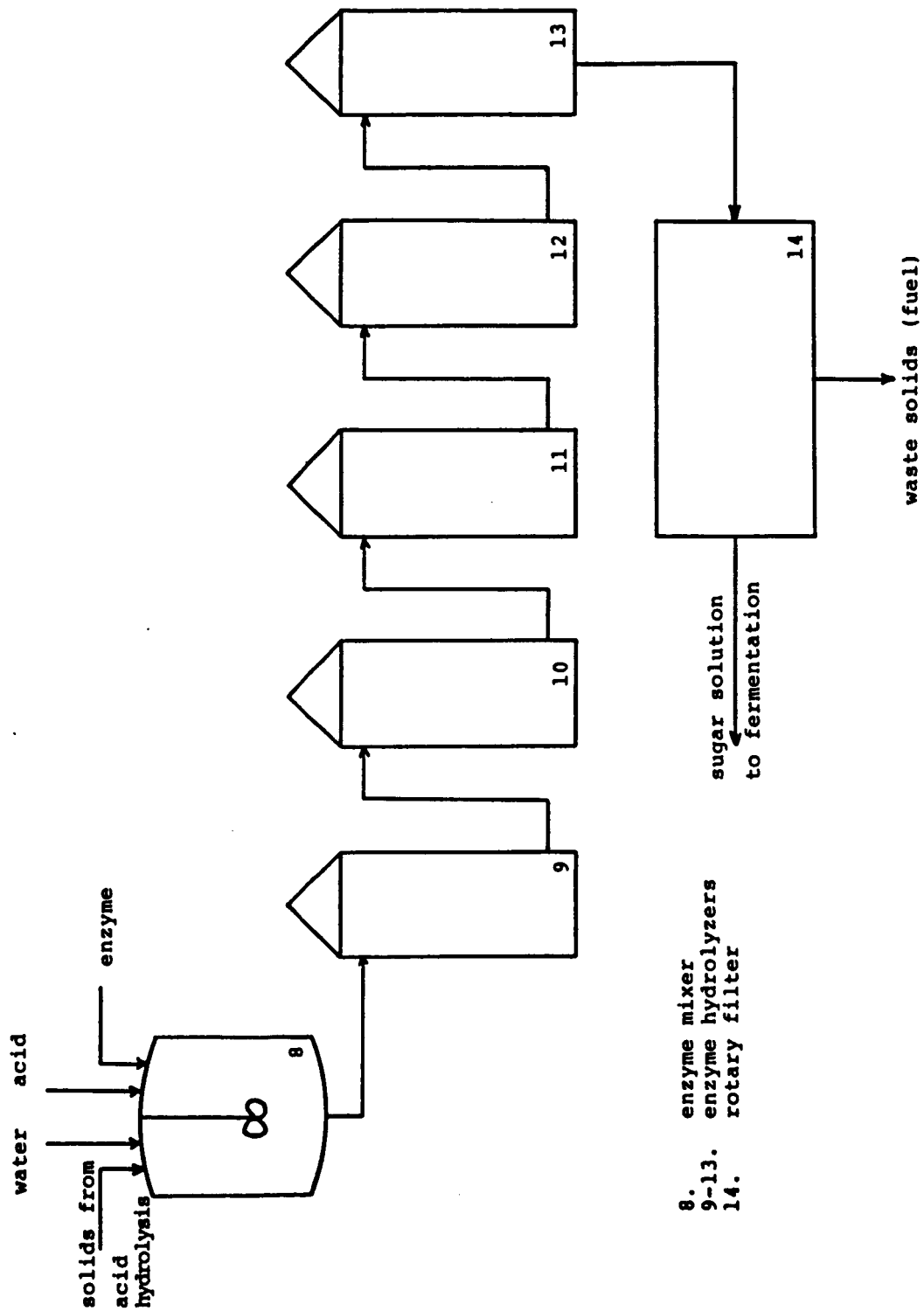
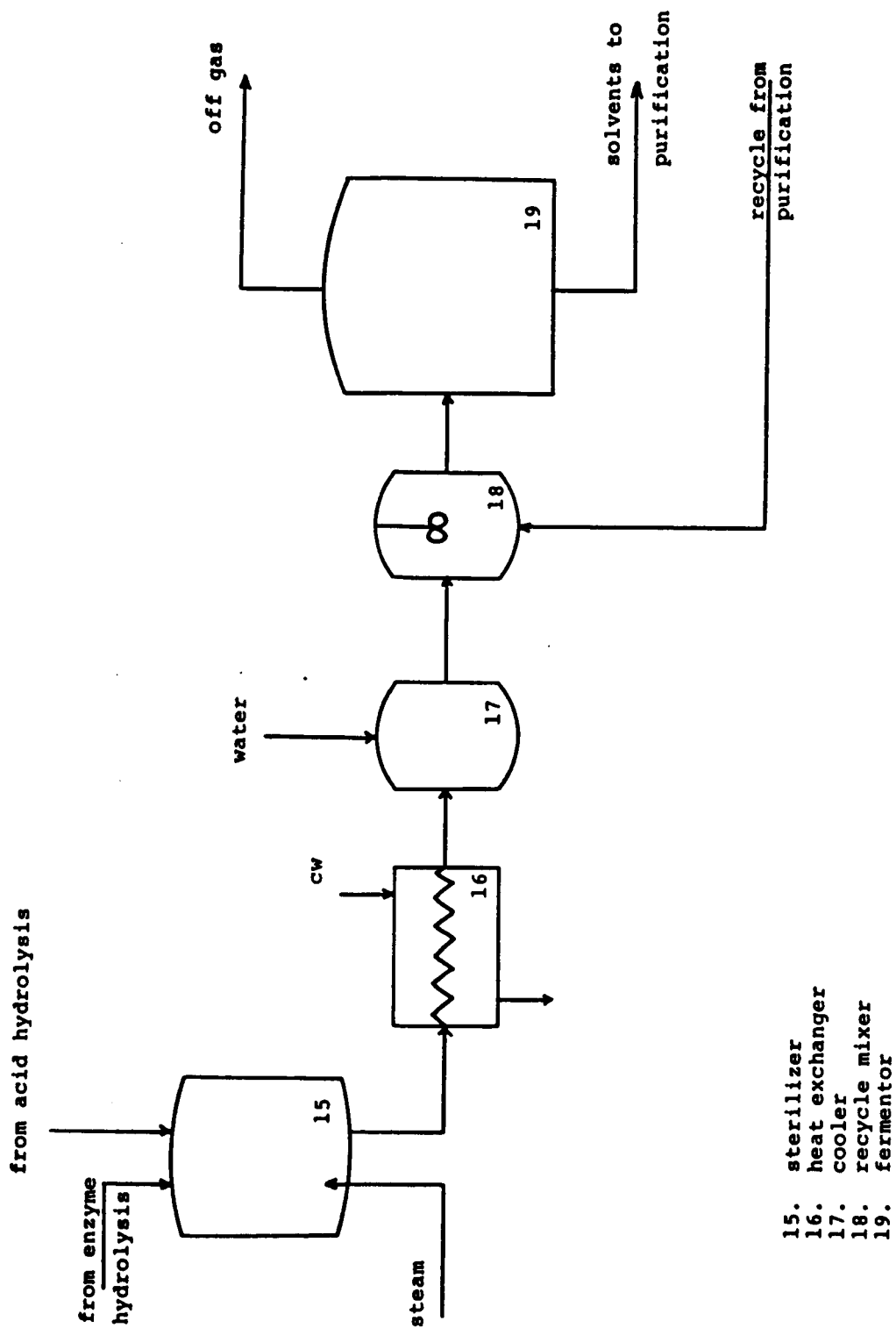


Figure 4.6 Enzyme Hydrolysis



- 15. sterilizer
- 16. heat exchanger
- 17. cooler
- 18. recycle mixer
- 19. fermentor

Figure 4.7 Fermentation

lignin , passed through a carbon column for purification purposes, and sent on to the fermentation section.

The unconverted celluloses and lignin from acid hydrolysis is mixed with water, acid and enzyme , and introduced to the first of a train of enzyme hydrolyzers (Figure 4.6). These tanks are maintained at the appropriate conditions, and after a total residence time of about 50 hours, the product stream is filtered in a rotary filter. The filtrate is sent on to the fermentation section after removing the enzyme if desired, and the solids are used as fuel.

In the fermentation section (Figure 4.7) the two streams from the two hydrolysis steps are sterilized by steam injection, and then cooled down to the temperature required for fermentation. The off-gas generated from the fermentors are compressed to facilitate carbon dioxide removal. The liquid product stream is sent to the purification section (see Figure 4.3), and the recycle is fed back into the reflux mixer. A portion of this stream is also purged, so that there is no buildup of biomass.

4.5 Costing of the ABE Process

ASPEN uses cost correlations which were produced by regression on cost data for a large number of equipment classes. Occasionally, the data was divided into groups to obtain a better fit. Extrapolations, whenever required, are based on the correlation variable. There are four modes available for costing:

- (i) Stand-alone
- (ii) Unit Operation (UOS) Reference
- (iii) User Correlation

(iv) User-supplied Cost

For the ABE costing, the stand-alone costing option was used. Thus, all design parameters required by the cost models were specified, as were utility capacities. The calculations of capital investment and operating cost requires the specification of numerous cost parameters, or the use of ASPEN defaults for the same. The defaults were used in most instances. The cost indices used were as follows:

Index	Value
Plant	325.0
Equipment	346.7
Labor	264.9

In addition, the labor rates assumed were \$ 13.75/hr.

Equipment costs for the entire ABE plant are shown in Table 4.3. ASPEN defaults have been used to evaluate these costs, except for the user-specified scale-up and adjustment factors, and in certain cases, the material factor. Table 4.4 shows the installation and utility costs for the base case ABE simulation. As far as equipment costs are concerned, the fermentation section requires the most capital: about 70 percent of the total investment is used here. The costs in this section are large mainly because the fermentation tanks are extremely large, and a large number of them are required to keep the plant in operation on a continuous basis.

The major utility requirements are of cooling water and steam. The largest costs (58 percent of total utility costs) are associated with the cooling water requirements in the fermentation step. Since the heat evolved in this step is of a very low

Table 4.3 Equipment Costs, Base Case ABE Plant
(thousand dollars)

EQUIPMENT	NO.	TOTAL PRICE	
Acid Hydrolysis:			
Crusher	2	341.4	
Slurry pump	2	105.5	
Slurry tank	1	43.5	
Acid hydrolyzer	1	72.6	
Quench tank	1	79.4	
Carbon column	1	51.8	
Centrifuge	1	149.6	
Pumps	10	65.4	
			909.2
Enzyme Hydrolysis:			
Mixing tank	1	33.5	
Enzyme hydrolyzers	5	11,539.2	
Rotary filter	1	76.6	
Pumps	10	65.4	
			11,714.7
Fermentation:			
Sterilizer	1	76.9	
Heat exchanger	12	1,090.1	
Cooling tank	1	102.4	
Fermentor	10	69,790.3	
Pumps	17	355.0	
			71,414.7
Purification:			
Column 1	1	191.0	
Column 2	1	145.4	
Column 3	1	299.2	
Column 4	1	193.4	
Column 5	1	299.2	
Column 6	1	299.2	
Evaporator	1	4,787.5	
Pumps	6	20.4	
			6,235.3
Carbon dioxide recovery:			
Compressors	2	7,147.8	
Pressure vessel	1	261.7	
			7,409.5
Storage:			
Solid (yard/building)	1	194.5	
Liquid (low pressure tanks)	6	3,428.0	
Gas (high pressure tanks)	2	868.4	
			4,490.4

Table 4.4(a) Installation Cost Summary, Base Case ABE Simulation
(thousand dollars)

SECTION	EQUIP. COST	MATERIAL COST	LABOR COST
ACID HYDROLYSIS	909	679	360
ENZYME HYDROLYSIS	11,715	2,065	1,190
FERMENTATION	71,415	24,092	15,624
PURIFICATION	6,235	1,393	736
CO ₂ RECOVERY	7,410	4,426	1,960
PRODUCT/RAW MATERIAL STORAGE	4,491	1,771	1,071
TESTING LABOR	---	---	2,946
CAPITALIZED SPARES	---	2,403	---
TOTAL	102,175	36,829	23,887

Table 4.4(b) Utility Cost Summary for Base Case ABE Simulation
(thousand dollars per year)

SECTION	ELECTRICITY	STEAM	WATER	REFRIG.
ACID HYDROLYSIS	207	30,548	644	---
ENZYME HYDROLYSIS	53	---	2,807	---
FERMENTATION	114	11,606	107,696	---
PURIFICATION	27	5,536	19,439	---
CO ₂ RECOVERY	---	---	---	5,112
TOTAL	401	47,690	130,586	5,112

quality (fermentation occurs at 33 degrees C), the water requirements are excessively large; any means of lowering these costs should be investigated. It should be mentioned here that it is probably more economical to set up a cooling tower in an actual plant, so that the water costs are not prohibitively large. This was not done in the current simulation because of the absence of a module for a cooling tower in the ASPEN program.

The capital investment report and the operating cost summary for this case are shown in Tables 4.5 and 4.6, which are taken from the actual ASPEN output report. In Table 4.6, the individual raw material and utility figures are not accurate, though the sum of the two numbers is. This is because some utilities (such as cooling water in the fermentors) were treated as inputs (and hence raw materials) to the system. Obviously, the economics do not change because of this.

All costs calculated for Table 4.6 were based on ASPEN defaults. The hourly rate for operating labor was taken as \$ 13.75, and the number of operators required per shift was estimated as 15. The depreciation method used was straight-line, with the plant life for tax purposes being taken as 15 years. The net operating cost of roughly \$ 253 million per year does not take into account the by-product credit accrued because of acetone and ethanol sales. If these are also taken into account, the cost of production of butanol works out to be \$ 0.84/Kg (roughly \$ 2.55 per gallon), as opposed to the September 1985 selling price (20) of \$ 0.79/Kg (about \$ 2.40 per gallon). There is some question as to whether all the by-products (such as acetic acid, butyric acid, acetoin, lignin, carbon-dioxide, etc.) can be sold. If it is

Table 4.5 Capital Investment Report, Base Case

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ABE COSTING
ECONOMIC EVALUATION SECTION

CAPITAL INVESTMENT REPORT
ASPEN METHOD

• PROJECT CONSTRUCTION COSTS FOR LOCATION, 1985 QUARTER : 1 **

	MATERIAL COST	LABOR COST	LABOR HOUR
PROCESS UNITS	\$ 138,643,775	\$ 23,886,941	1,737,232
UTILITY UNITS	0	0	0
RECVNG , SHIPPING & STOR	0	0	0
SERVICE BUILDING	11,390,061	3,361,163	244,448
SERVICE SYST & DISTRBUTN	7,714,915	1,927,067	140,150
ADDITIONAL DIRECT	0	0	0
SUBTOTAL	\$ 157,748,751	\$ 29,175,172	2,121,831
SITE DEVELOPMENT	1,730,530	34,045	2,476
FREIGHT	3,334,986		
TOTAL DIRECT COST	\$ 162,814,267	\$ 29,209,217	2,124,307
FIELD INDIRECT	7,886,488	21,322,728	1,292,287
FIELD CONSTR COST	\$ 170,700,756	\$ 50,531,945	
FIELD CONSTR LAB HRS			3,416,593

• PROJECT FIXED INVESTMENT FOR LOCATION, 1985 QUARTER : 1 **

TOTAL FIELD CONSTRUCTION COST		\$ 221,232,700
PROJECT MANAGEMENT COST	\$ 14,104,994	
ENGINEERING & HOME OFFICE COST	28,209,988	
FEES, PERMITS & INSURANCE	18,806,659	
ADDITIONAL DEPRECIABLE COST	0	
SUBTOTAL - INDIRECTS		61,121,640
TOTAL DEPRECIABLE (EX. CONT.)		\$ 282,354,341
PROCESS CONTINGENCY	\$ 56,470,868	
PROJECT DEFINITION CONTINGENCY	28,235,434	
TOTAL CONTINGENCY		84,706,302
TOTAL DEPRECIABLE CAPITAL		\$ 367,060,643
LAND	\$ 7,770,194	
ROYALTY & EXPENSES	0	
ADDITIONAL NON-DEPRECIABLE	0	
SUBTOTAL (NON-DEPRECIABLE COSTS)		7,770,194
TOTAL FIXED INVESTMENT		\$ 374,830,837

Table 4.6 Annual Operating Cost, Base Case

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ABE COSTING

ECONOMIC EVALUATION SECTION

ANNUAL OPERATING COST

(1985\$, CAPACITY RATIO: 1.00)

TOTAL RAW MATERIAL		\$	235,892,050
TOTAL UTILITIES			25,377,712
OPERATING LABOR (131490 HR)			1,807,987
MAINTENANCE LABOR (1008173 HR)	\$	13,862,388	
MAINTENANCE MATERIAL		9,324,233	
SUB-TOTAL MAINTENANCE			23,186,621
SUPERVISION			3,134,075
FRINGE BENEFITS			7,521,780
OPERATING SUPPLIES			182,416
OTHER DIRECT COST			0
TOTAL DIRECT COST	\$		298,242,306
PROPERTY TAX	\$	7,770,194	
PROPERTY INSURANCE		3,108,078	
ADMINST. & GENERAL		11,383,563	
DEPRECIATION (STRAIGHT LINE)		25,900,648	
TOTAL INDIRECT COST			48,162,483
GROSS OPERATING COST	\$		346,404,789
LESS: BY-PRODUCT CREDIT			93,044,428
NET OPERATING COST	\$		253,360,361
SUMMARY:			
FIXED COST	\$	83,995,363	
VARIABLE COST		262,409,426	
TOTAL GROSS OPERATING COST	\$		346,404,789
GROSS COST EXCL. DEPRECIATION	\$		320,504,141

assumed that only acetone and ethanol can be sold, the cost of production of butanol is then \$1.21/Kg (or \$3.68 per gallon). It would be reasonable to assume that the cost of production would be somewhere between \$0.84/Kg and \$1.21/Kg, making this method an unattractive way of manufacturing butanol. It should be noted here however, that some major costs (such as cooling water and other utility costs) could conceivably be reduced by some better design concepts (such as energy integration, or the building of a cooling tower, etc.). The cost of production then would be significantly lower.

4.6 Changes to the Basic Flowsheet

Table 4.4 shows that the major utility cost is the cooling water cost in the fermentation section of the plant, and may be as much as 42.5 percent of the annual net operating cost (see Table 4.6). It would therefore be obvious that any changes made to the flowsheet should be geared towards investigating methods of reducing these costs. Before that is done, it would be useful to see why these costs are so large.

One advantage of continuous or semi-continuous processing in the case of ABE fermentations is that butanol, which is an inhibitor of the fermentation, may be continually removed from the product stream. This allows for a recycle of unconverted reactants, and a feed sugar concentration larger than that originally thought possible. There are two negative effects of this, however. The first is a result of the separation scheme, which is distillation in this case. Live steam is added in the first column, thereby bringing temperatures up to levels where

separation of the products from water may occur: this results in further dilution of the recycle stream, and an extra cooling cost because the temperature of this stream (about 100 degrees C) must be brought down to the fermentation temperature (33 degrees C). The second negative effect is that the fermentor sizes have to be increased, because the recycle stream is less concentrated in the sugars than the streams coming from the hydrolysis steps.

One relatively easy way of handling this problem would be to concentrate the recycle stream by evaporating off most of the water. However, this would be too costly in terms of equipment costs as well as high pressure steam requirements. Another way would be to investigate possibilities of having more concentrated feeds to the fermentation section, by altering some operating conditions further upstream. Two schemes were explored, and are explained here.

A. Concentrated Feed to Enzyme Hydrolyzers

Literature surveys have shown that most enzyme hydrolysis studies have been carried out at a maximum initial cellulose concentration of about 8 weight percent. Lee and Fan (21) mention that at above these concentrations, the cellulose fibers form a network which entraps water and renders it less movable, thereby hindering the hydrolysis. Particle sizes in their case was of the order of 0.04 mm, and the substrate involved was Solka Floc. Since the problem seems to be a physical one, and since our simulation is for roughly 2 mm particle sizes, it seems that the problem may not be as acute in this case. Also, the substrate is acid-hydrolyzed wood, and the 'netting' effect would probably not be seen. There has been mention in the literature (22, 23) of

substrate inhibition, but the data is not extensive. In any event, it is a worthwhile exercise to gauge the effect of having higher feed concentrations to the enzyme hydrolysis step on the entire process economics, if only to answer a 'what if' question. If the improvement in the economics was substantial enough, a potential area of research would be identified.

As opposed to the base case of 8 wt % substrate concentration in the inlet to enzyme hydrolysis, a simulation with roughly 26 wt % was done. This had far-reaching effects on the process economics, ranging from different utility costs (because of lower steam requirements for heating during hydrolysis and for sterilization prior to fermentation, and of lower cooling costs during fermentation) to lower equipment costs (because of the lower throughputs). An overall view of the economics can be found in Tables 4.7 and 4.8, which are the capital investment report and the annual operating cost respectively.

B. Two-Stage Acid Hydrolysis

Since there is some question as to whether enzyme hydrolysis can proceed at high inlet substrate concentrations, an alternative is to carry out the hydrolysis in two stages. The amorphous cellulose and hemicellulose fractions could be hydrolyzed as before, and the remaining insoluble crystalline fraction could be hydrolyzed by hydrolysis at other conditions. Care can be taken to ensure the degradation reactions do not proceed beyond tolerable levels. However, the overall yield of the two-step process will not be as good as the combination of acid and enzyme hydrolysis because of some unavoidable product degradation.

Table 4.7 Capital Investment Report, Case A

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ABE COSTING

ECONOMIC EVALUATION SECTION

CAPITAL INVESTMENT REPORT
ASPEN METHOD

* PROJECT CONSTRUCTION COSTS FOR LOCATION, 1985 QUARTER : 1 **

	MATERIAL COST	LABOR COST	LABOR HOUR
PROCESS UNITS	\$ 73,754,695	\$ 13,197,361	959,808
UTILITY UNITS	0	0	0
RECVNG , SHIPPING & STOR	0	0	0
SERVICE BUILDING	6,091,274	1,797,511	130,728
SERVICE SYST & DISTRBUTN	4,125,847	1,030,573	74,951
ADDITIONAL DIRECT	0	0	0
SUBTOTAL	\$ 83,971,816	\$ 16,025,446	1,165,487
SITE DEVELOPMENT	925,468	18,207	1,324
FREIGHT	1,783,512		
TOTAL DIRECT COST	\$ 86,680,795	\$ 16,043,652	1,166,811
FIELD INDIRECT	4,331,786	11,711,866	709,810
FIELD CONSTR COST	\$ 91,012,581	\$ 27,755,519	
FIELD CONSTR LAB HRS			1,876,621

* PROJECT FIXED INVESTMENT FOR LOCATION, 1985 QUARTER : 1 **

TOTAL FIELD CONSTRUCTION COST		\$ 118,768,100
PROJECT MANAGEMENT COST	\$ 7,593,936	
ENGINEERING & HOME OFFICE COST	15,187,872	
FEES, PERMITS & INSURANCE	10,125,248	
ADDITIONAL DEPRECIABLE COST	0	
SUBTOTAL - INDIRECTS		32,907,057
TOTAL DEPRECIABLE (EX. CONT.)		\$ 151,675,157
PROCESS CONTINGENCY	\$ 30,335,031	
PROJECT DEFINITION CONTINGENCY	15,167,516	
TOTAL CONTINGENCY		45,502,547
TOTAL DEPRECIABLE CAPITAL		\$ 197,177,704
LAND	\$ 4,183,367	
ROYALTY & EXPENSES	0	
ADDITIONAL NON-DEPRECIABLE	0	
SUBTOTAL (NON-DEPRECIABLE COSTS)		4,183,367
TOTAL FIXED INVESTMENT		\$ 201,361,071

Table 4.8 Annual Operating Cost, Case A

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ARE COSTING
ECONOMIC EVALUATION SECTION

ANNUAL OPERATING COST

(1985\$, CAPACITY RATIO: 1.00)

TOTAL RAW MATERIAL		\$	158,967,229
TOTAL UTILITIES			25,340,827
OPERATING LABOR (131490 HR)			1,807,987
MAINTENANCE LABOR (542786 HR)	\$	7,463,321	
MAINTENANCE MATERIAL		5,020,040	
SUB-TOTAL MAINTENANCE			12,483,360
SUPERVISION			1,854,262
FRINGE BENEFITS			4,450,228
OPERATING SUPPLIES			182,416
OTHER DIRECT COST			0
TOTAL DIRECT COST	\$		205,760,586
PROPERTY TAX	\$	4,183,367	
PROPERTY INSURANCE		1,673,347	
ADMINST. & GENERAL		6,735,035	
DEPRECIATION (STRAIGHT LINE)		13,944,555	
TOTAL INDIRECT COST			26,536,303
GROSS OPERATING COST	\$		232,296,889
LESS: BY-PRODUCT CREDIT			106,004,187
NET OPERATING COST	\$		126,292,701
			=====
SUMMARY:			
FIXED COST	\$	47,314,556	
VARIABLE COST		184,982,333	
TOTAL GROSS OPERATING COST	\$		232,296,889
GROSS COST EXCL. DEPRECIATION	\$		218,352,334

Tables 4.9 and 4.10 present the capital investment report and annual operating cost for this case. Again, there were improvements in the economics. These were substantial when compared to the base case, but not as dramatic when compared to Case A above. An extra cost is introduced because of the steam requirements for the second acid hydrolysis, but this is more than offset by the savings in cooling water requirements in the fermentation stage. The desired product yields were lower in this case.

Table 4.11 compares installation costs and utility costs for each of the three cases. The dramatic improvement in the cost of the fermentation section is not matched by similar improvements in any other section. For Case B, there is a significant reduction in costs when the second hydrolysis section is compared to the previous enzyme hydrolysis costs. Additionally, some real improvements that are not reflected in the costs are that in Case B, an extra species (enzyme) is not being introduced into the system. Therefore, enzyme recovery and production costs would be saved. In terms of \$/Kg, the cost of production of butanol works out to be as follows, assuming all the acetone and ethanol that is produced in each case is sold:

	with by-product credit	without by-product credit
Base Case	0.84	1.21
Case A	0.35	0.81
Case B	0.23	0.83

These costs obviously do not include the effects of certain

Table 4.9 Capital Investment Report, Case B

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ABE COSTING
ECONOMIC EVALUATION SECTION

CAPITAL INVESTMENT REPORT
ASPEN METHOD

* PROJECT CONSTRUCTION COSTS FOR LOCATION, 1985 QUARTER : 1 **

	MATERIAL COST	LABOR COST	LABOR HOUR
PROCESS UNITS	\$ 62,063,136	\$ 11,642,432	846,722
UTILITY UNITS	0	0	0
RECVNG , SHIPPING & STOR	0	0	0
SERVICE BUILDING	5,147,190	1,518,916	110,467
SERVICE SYST & DISTRBUTN	3,486,384	870,845	63,334
ADDITIONAL DIRECT	0	0	0
SUBTOTAL	\$ 70,696,710	\$ 14,032,193	1,020,523
SITE DEVELOPMENT	782,030	15,385	1,119
FREIGHT	1,507,086		
TOTAL DIRECT COST	\$ 72,985,826	\$ 14,047,578	1,021,642
FIELD INDIRECT	3,792,846	10,254,732	621,499
FIELD CONSTR COST	\$ 76,778,672	\$ 24,302,311	
FIELD CONSTR LAB HRS			1,643,141

* PROJECT FIXED INVESTMENT FOR LOCATION, 1985 QUARTER : 1 **

TOTAL FIELD CONSTRUCTION COST	\$ 101,080,983
PROJECT MANAGEMENT COST	\$ 6,475,819
ENGINEERING & HOME OFFICE COST	12,951,637
FEES, PERMITS & INSURANCE	8,634,425
ADDITIONAL DEPRECIABLE COST	0
SUBTOTAL - INDIRECTS	28,061,880
TOTAL DEPRECIABLE (EX. CONT.)	\$ 129,142,863
PROCESS CONTINGENCY	\$ 25,828,573
PROJECT DEFINITION CONTINGENCY	12,914,286
TOTAL CONTINGENCY	38,742,859
TOTAL DEPRECIABLE CAPITAL	\$ 167,885,722
LAND	\$ 3,567,415
ROYALTY & EXPENSES	0
ADDITIONAL NON-DEPRECIABLE	0
SUBTOTAL (NON-DEPRECIABLE COSTS)	3,567,415
TOTAL FIXED INVESTMENT	\$ 171,453,137

Table 4.10 Annual Operating Cost, Case B

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 ABE COSTING
 ECONOMIC EVALUATION SECTION

ANNUAL OPERATING COST

(1985\$, CAPACITY RATIO: 1.00)

TOTAL RAW MATERIAL		\$	150,264,848
TOTAL UTILITIES			25,309,404
OPERATING LABOR (131490 HR)			1,807,987
MAINTENANCE LABOR (462867 HR)	\$	6,364,434	
MAINTENANCE MATERIAL		4,280,898	
SUB-TOTAL MAINTENANCE			10,645,333
SUPERVISION			1,634,484
FRINGE BENEFITS			3,922,763
OPERATING SUPPLIES			182,416
OTHER DIRECT COST			0
TOTAL DIRECT COST	\$		194,361,593
PROPERTY TAX	\$	3,567,415	
PROPERTY INSURANCE		1,426,966	
ADMINST. & GENERAL		5,936,762	
DEPRECIATION (STRAIGHT LINE)		11,891,384	
TOTAL INDIRECT COST			22,822,526
GROSS OPERATING COST	\$		217,184,119
LESS: BY-PRODUCT CREDIT			125,530,452
NET OPERATING COST	\$		91,653,667
SUMMARY:			
FIXED COST	\$	41,015,509	
VARIABLE COST		176,168,610	
TOTAL GROSS OPERATING COST	\$		217,184,119
GROSS COST EXCL. DEPRECIATION	\$		205,292,735

Table 4.11 (a) Comparison of Installation Costs, Three Cases
(thousand dollars)

SECTION	BASE CASE	CASE A	CASE B
ACID HYDROLYSIS	1948	1948	1948
ENZYME HYDROLYSIS*	14,970	11,454	2,155
FERMENTATION	111,131	41,621	36,407
PURIFICATION	8,365	8,365	8,365
CO ₂ RECOVERY	13,796	13,796	13,796
PRODUCT/RAW MATERIAL STORAGE	7,333	7,142	8,843
TESTING LABOR	2,946	1,576	1,333
CAPITALIZED SPARES	2,403	1,051	860
TOTAL	162,892	86,953	73,707

Table 4.11 (b) Comparison of Total Utility Costs, Three Cases
(thousand dollars)

SECTION	BASE CASE	CASE A	CASE B
ACID HYDROLYSIS	31,399	31,399	31,399
ENZYME HYDROLYSIS*	2,860	173	10,414
FERMENTATION	119,416	45,462	33,557
PURIFICATION	25,002	25,002	25,002
CO ₂ RECOVERY	5,112	5,112	5,112
TOTAL	183,789	107,148	105,484

* For Case B, these are costs for the second acid hydrolysis stage

factors such as fermentor contamination. Also, since no standby equipment have been accounted for, costs would be higher.

Taking the selling price to be 0.79/Kg, the target cost of production should be around 0.69/Kg, so that a return of 15 percent is made on investments. It would seem therefore, that both Case A and Case B might be viable candidates for further study. At the present time, both cases have associated difficulties. For Case A, the problem is whether the enzyme hydrolyzers can handle higher substrate concentrations than 8 weight percent. For Case B, the uncertainty is in knowing whether the acid hydrolyzers which have worked in the bench scale will work in the enormous scales envisaged for this simulation.

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APPENDIX A

FORTRAN Listings of User Files

This appendix contains the listings of the user files created to enable the simulation of the A-B-E Process. There are four subroutines, each written according to the guidelines in the ASPEN manuals. Descriptions of the input parameters are included as comment statements at the beginning of each subroutine. The four subroutines do the following:

NAME	DESCRIPTION
USR001	Enzyme hydrolyzer
USR002	Acid hydrolyzer
USR003	A-B-E Fermentor
USR004	Sterilizer

```

      SUBROUTINE USR001(NSIN ,NINFI ,SIN1 ,SIN2 ,SIN3 ,SIN4 ,
1          SINFI ,NSOUT ,NINFO ,SOUT1 ,SOUT2 ,SOUT3 ,SOUT4 ,
2          SINFO ,NSUBS ,IDXSUB,ITYPE ,NINT ,INT ,NREAL ,
3          REAL ,IDS ,NPO ,NBOPST,NIW ,IW ,NW ,
4          W ,NSIZE ,SIZE)
C*****
C CHANGE #1 (10/02/85): Sign corrected on outlet heat stream
C
C This subroutine is the first version of an enzyme hydrolyzer
C Currently (7/12/85) it handles only one input and one output
C stream of stream class MIXEDNC. Additionally, some require-
C are as follows:
C
C (1) The component lists have to be in the following order:
C     CONVENTIONAL: water
C     NONCONVEN   : crystalline cellulose,amorphous cellu-
C                   lose,cellebiose,glucose and enzyme
C Additional components may be added to these lists as
C required.
C (2) SI units have been used.
C (3) Enzyme activity is taken is cellulase (FPU/mL) and
C cellobiase (BU/mL), and are the first two elements of the
C user-defined component attribute CAUSR1 of NC-component
C ENZYME.
C (4) Int(1): no. of records to be retained for results pass
C (5) Real(1) : lower limit for integration (hr)
C Real(2) : upper limit for integration (hr)
C Real(3) : temperature of hydrolyzer (K)
C Real(4) : pressure of hydrolyzer (Pa)
C (6) In addition to these 4 spaces for the real vector, space
C must be kept to store profiles for the results pass.
C The additional spaces must equal at least 5*(int(1) + 1)
C in number.
C (7) The dimension of RETN has to be 6*NCC + 37
C
C The kinetics for this subroutine are taken from:Peitersen &
C Ross, B & B, 21, 997 (1979).
C
C Subroutines called are: GEAR, RPTHDR, USRCPY, FLASH
C
C*****
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION SIN1(1) ,SIN2(1) ,SIN3(1) ,SIN4(1) ,
1          SINFI(1) ,SOUT1(1) ,SOUT2(1) ,SOUT3(1) ,
2          SOUT4(1) ,SINFO(1) ,IDXSUB(NSUBS),ITYPE(NSUBS) ,
3          INT(NINT) ,REAL(NREAL),IDS(2,13) ,NBOPST(3,NPO),
4          IW(NIW) ,W(NW) ,SIZE(NSIZE) ,WS(68) ,
5          A(32) ,XOUT(100) ,Y(4) ,RETN(103) ,
6          IRETN(6)
      COMMON /USER/ RMISS ,IMISS ,NGBAL ,IPASS ,IRESTR ,ICONVG,
1          LMSG ,LPMSG ,KFLAG ,NHSTRY ,NRPT ,NTRMNL,
2          ISIZE
      COMMON /NCOMP/ NCC ,NNCC
      COMMON /IDSCC/ IDSCC(2,1)
      COMMON /IDSNCC/ IDSNCC(2,1)
      COMMON /IDXCC/ IDXCC(1)
      COMMON /IDXNCC/ IDXNCC(1)
      COMMON /MW/ XMW(1)
      COMMON /RPTGLB/ IREPFL,ISUB(10)

```

```

C      The next two lines are for GEAR's benefit
C
COMMON /GEARLC/ XDUMB(70),IDUMB(84)
DATA N,TEST1,TEST2,EPS,NWS,NA/4,1D-10,1D0,.1D0,68.32/
DATA KODE,NPKODE,KPHASE,MXIT,ETOL,KRSLT/2,2,0,30,1D-4,2/

C
C      Go to 500 for Results pass
C
      IF (IPASS.EQ.4) GO TO 500
      L = 0
      NOUT = - INT(1)
      TEMP = REAL(3)
      PRES = REAL(4)

C
C      Store initial values, and convert inlet flowrates (SI) to
C      concentrations (g/L)
C
      HO = SIN1(1)*XMW(1)
      CCO = SIN1(NCC + 10)
      ACO = SIN1(NCC + 11)
      CLO = SIN1(NCC + 12)
      GCO = SIN1(NCC + 13)
      T = 1D3/HO
      Y(1) = CCO*T
      Y(2) = ACO*T
      Y(3) = CLO*T
      Y(4) = GCO*T

C
C      Extract cellulase and cellobiase activities
C
      CLLASE = SIN1(NCC + NNCC + 19)
      CLBASE = SIN1(NCC + NNCC + 20)

C
C      X and XEND are the limits of the integration, passed from the
C      input file
C
      X = REAL(1)
      XEND = REAL(2)
      JFLAG = 0
      IFLAG = 0
10    CONTINUE
      IF (IFLAG.EQ.1) GO TO 12
      DO 11 I = 1,N
        IF (Y(I).LE.1D-3) THEN
          TEST1 = 1D0
          TEST2 = 0D0
          IFLAG = 1
        END IF
11    CONTINUE
12    CONTINUE
      CALL GEAR(N,X,XEND,Y,TEST1,TEST2,EPS,NOUT,XOUT,NWS,WS,NA,A,
1      JFLAG,H,NSTEP,IORDER,NDERIV)
      IF (JFLAG) 900,910,20
      GO TO (30,40,10) JFLAG

20    C
C      Evaluate the reaction rates and derivative values
C
30    CONTINUE
      DO 35 I = 1,N
        IF (Y(I).LE.1D-8) Y(I) = 0D0

```

```

35      CONTINUE
      RATE1 = 0.959*Y(1)*CLLASE/(2.14 + Y(1) + 46.5*Y(2))
      RATE2 = 31.3*Y(2)**.6*CLLASE/(30.4 + Y(2) + 9.74*Y(3))
      RATE3 = 3.58*Y(3)*CLBASE/(0.265 + Y(3) + 0.376*Y(4))
      RATE4 = 4.12*Y(2)*CLLASE/(44.1 + Y(2) + 2.25*Y(4))
      IF (RATE1.LE.1D-8) RATE1 = 0D0
      IF (RATE2.LE.1D-8) RATE2 = 0D0
      IF (RATE3.LE.1D-8) RATE3 = 0D0
      IF (RATE4.LE.1D-8) RATE4 = 0D0
      WS(1) = - RATE1
      WS(2) = RATE1 - RATE2 - RATE4
      WS(3) = RATE2 - RATE3
      WS(4) = RATE3 + RATE4
      GO TO 10
40      TYPE *,X,Y
100     FORMAT(1X,6D13.5,3I7)
C
C      Store values for results pass
C
      REAL(5*L + 5) = X
      DO 45 I = 1,4
        IF (Y(I).LE.1D-10) Y(I) = 0D0
        J = 5*L + I + 5
        REAL(J) = Y(I)
45      CONTINUE
      L = L + 1
      GO TO 10
900     WRITE(NTRMNL,200),JFLAG
200     FORMAT(1X,'INTEGRATION HALTED BECAUSE OF ERROR CONDITION '13)
      GO TO 999
910     WRITE(NTRMNL,300)
300     FORMAT(1X,'INTEGRATION COMPLETED SUCCESSFULLY')
C
C      Copy inlet stream into outlet stream
C
      CALL USRCPY(IDS(1,1),1,1,NSIN,NSOUT)
C
C      Copy the results from GEAR into the outlet stream
C
      T = 1D0/T
      S = 0D0
      DO 160 I = 1,4
        Y(I) = Y(I)*T
        SOUT1(NCC + I + 9) = Y(I)
        S = S + Y(I)
160     CONTINUE
      SOUT1(1) = (CC0 + AC0 + CL0 + GC0 + H0 - S)/XMW(1)
      N1 = NCC + 1
      SOUT1(N1) = 0D0
      DO 170 I = 1,NCC
        SOUT1(N1) = SOUT1(N1) + SOUT1(I)
170     CONTINUE
      N1 = NCC + 9
      N2 = N1 + NNCC + 1
      SOUT1(N2) = 0D0
      DO 180 I = 1,NNCC
        SOUT1(N2) = SOUT1(N2) + SOUT1(N1 + I)
180     CONTINUE
      SOUT1(NCC + 2) = TEMP
      SOUT1(NCC + 3) = PRES

```

```

SOUT1(NCC + NNCC + 11) = TEMP
SOUT1(NCC + NNCC + 12) = PRES
C
C
C
Flash the outlet stream to find energy requirements
CALL FLASH(SOUT1 ,NSUBS ,IDXSUB,ITYPE ,NBOPST,KODE ,NPKODE,
1      KPHASE,MXIT ,ETOL ,TEMP ,PRES ,GUESS ,LMSG ,
2      LPMSG ,IRESTR,KRSLT ,RETN ,IRETN ,LCFLAG)
IF (LCFLAG.NE.0) WRITE(NTRMNL,950) LCFLAG
950  FORMAT(1X,'FLASH DID NOT CONVERGE. LCFLAG = ',11)
N1 = NCC + NNCC + 9
SINFO(1) = -((SOUT1(NCC + 1)*SOUT1(NCC + 9)*SOUT1(NCC + 4) +
1      SOUT1(N1 + 1)*SOUT1(N1 + 4)) - (SIN1(NCC + 1)*
2      SIN1(NCC + 9)*SIN1(NCC + 4) + SIN1(N1 + 1)*
3      SIN1(N1 + 4)))
GO TO 999
C
C
C
The following is the report writing section
500  CONTINUE
II = (INT(1) + 1) + 25
CALL RPTHDR(II,0,3,ISUB)
WRITE(NRPT,920)
WRITE(NRPT,930),((IDSNCC(1,I),IDSNCC(2,I)),I=1,4)
920  FORMAT(/20X,'PROFILES (G/L) ARE AS FOLLOWS: '/')
930  FORMAT(8X,'TIME',9X,2A4,6X,2A4,6X,2A4,6X,2A4/)
WRITE(NRPT,940), (REAL(J), J=5,5*(INT(1)+1)+4)
940  FORMAT(2X,5D14.5)
999  RETURN
END

```

```

      SUBROUTINE USR002(NSIN ,NINFI ,SIN1 ,SIN2 ,SIN3 ,SIN4 ,
1          SINFI ,NSOUT ,NINFO ,SOUT1 ,SOUT2 ,SOUT3 ,SOUT4 ,
2          SINFO ,NSUBS ,IDXSUB,ITYPE ,NINT ,INT ,NREAL ,
3          REAL ,IDS ,NPO ,NBOPST,NIW ,IW ,NW ,
4          W ,NSIZE ,SIZE)
C*****
C CHANGE #5: (9/24/85) Avg mol wt. computed for outlet material stream*
C CHANGE #4: (9/24/85) H2O consumption based on total material balance*
C CHANGE #3: (9/20/85) Sign corrected on outlet heat stream *
C CHANGE #2: (9/20/85) GLO inserted to keep track of water consumption*
C CHANGE #1: (8/09/85) Kwarteng's kinetic parameters inserted *
C
C      This subroutine is the first version of an acid hydrolyzer *
C      Currently (7/11/85) it handles only one input and one output *
C      stream of stream class MIXEDNC. Some additional requirements*
C      are as follows:
C
C      (1) The component lists have to be in the following order: *
C           CONVENTIONAL: water, sulfuric acid, hmf, furfural *
C           NONCONVEN   : crystalline cellulose, amorphous cell- *
C                        ulose, cellobiose, glucose, enzyme, *
C                        hemicellulose, xylose and lignin *
C      Additional components may be added to these lists as *
C      required.
C      (2) SI units have been used
C      (3) Int(1): no. of records to be retained for results pass *
C           Int(2): id of substrate material
C                   1 : Douglas Fir
C                   2 : Kraft Paper
C                   3 : Solka Floc
C                   4 : Oak Sawdust
C                   5 : Corn Stover
C                   6 : Kwarteng's kinetic constants
C      (4) Real(1) : lower limit of integration (min)
C           Real(2) : upper limit of integration (min)
C           Real(3) : temperature of hydrolyzer (K)
C           Real(4) : pressure of hydrolyzer (Pa)
C      (5) In addition to these 4 spaces for the real vector, space*
C           must be kept to store profiles for the results pass.
C           The additional spaces must equal at least 7*(int(1) + 1)*
C           in number.
C
C      The kinetics for this routine are taken from Bhandari et al. *
C      B & B, 26, 320 (1984)
C      See also I. K. Kwarteng, PhD Thesis, Dartmouth College (1983)*
C
C      Subroutines called: GEAR, USRCPY, FLASH, RPTHDR
C
C*****
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION SIN1(1) ,SIN2(1) ,SIN3(1) ,SIN4(1) ,
1          SINFI(1) ,SOUT1(1) ,SOUT2(1) ,SOUT3(1) ,
2          SOUT4(1) ,SINFO(1) ,IDXSUB(NSUBS),ITYPE(NSUBS) ,
3          INT(NINT) ,REAL(NREAL),IDS(2,13) ,NBOPST(3,NPO),
4          IW(NIW) ,W(NW) ,SIZE(NSIZE) ,WS(68) ,
5          A(32) ,XOUT(100) ,Y(4) ,R1K0(6) ,
6          R1EXP(6) ,R1AE(6) ,R2K0(6) ,R2EXP(6) ,
7          R2AE(6) ,INDEX(1) ,RETN(61) ,IRETN(6)
      COMMON /USER/ RMISS ,IMISS ,NGBAL ,IPASS ,IRESTR ,ICONVG,
1          LMSG ,LPMSG ,KFLAG ,NHSTRY ,NRPT ,NTRMNL.

```

```

2          ISIZE
COMMON /NCOMP/ NCC ,NNCC
COMMON /IDSCC/ IDSCC(2,1)
COMMON /IDSNCC/ IDSNCC(2,1)
COMMON /IDXCC/ IDXCC(1)
COMMON /IDXNCC/ IDXNCC(1)
COMMON /MW/ XMW(1)
COMMON /RPTGLB/ IREPFL,ISUB(10)
COMMON /STWORK/ IDUM(14), MF, MX, MX1, MX2, MY, MCS, MNC,
1          IDUM1(4), MIM, MIC, MIN, IDUM2(17)
COMMON /STWKWK/ NCPM, NCPCS, NCPCNC, NTRIAL, IDUM3(2),TCALC,
1          PCALC, VCALC, QCALC, BETA, RDUM(21), RESULTS(1)
COMMON /GEARLC/ XDUMB(70),IDUMB(84)
EQUIVALENCE (INDEX(1),RESULTS(1))
DATA KODE,NPKODE,KPHASE,MXIT,ETOL,KRSLT/2,2,0,30,1D-4,2/
DATA N,TEST1,TEST2,EPS,NWS,NA,GC/4,1D-10,1D0,.1D0,68,32,1.9872D-3/
DATA R1K0/1.73D19,2.8D20,1.22D19,4.4D18,2.71D19,1.45D15/
DATA R2K0/2.38D14,4.9D14,3.79D14,2.8D12,2.01D14,3.84D9/
DATA R1EXP/1.34,1.78,1.16,1.0,2.74,1.157/
DATA R2EXP/1.02,0.55,0.69,1.8,1.86,0.569/
DATA R1AE/42.9,45.1,45.2,42.9,45.3,33.72/
DATA R2AE/32.87,32.8,32.8,30.0,32.8,20.99/

C
C      Go to 500 for Results pass
C
      IF (IPASS.EQ.4) GO TO 500
      L = 0
      NOUT = - INT(1)
      TEMP = REAL(3)
      PRES = REAL(4)

C
C      Find the total mass flow rate
C
      SUM = ODO
      DO 5 I = 1,NCC
        SUM = SUM + XMW(I)*SIN1(I)
5      CONTINUE
      DO 6 I = 1,NNCC
        SUM = SUM + SIN1(NCC + 9 + I)
6      CONTINUE

C
C      Find weight % of acid
C
      ACID = 100.*SIN1(2)*XMW(2)/SUM
      I = INT(2)
      GCTEMP = 1./(GC*TEMP)

C
C      Evaluate the pre-exponential factors of the reactions
C
      RK1 = R1K0(I)*ACID**R1EXP(I)*DEXP( - R1AE(I)*GCTEMP)
      RK2 = R2K0(I)*ACID**R2EXP(I)*DEXP( - R2AE(I)*GCTEMP)
      IF (I.LE.5) THEN
        RK3 = (7.64 - 3.68/ACID)*1D20*DEXP( - 41.*GCTEMP)
        RK4 = (4.60 - 1.95/ACID)*1D14*DEXP( - 32.*GCTEMP)
      ELSE
        RK3 = 6.24D13*ACID**1.1704*DEXP( - 27.83*GCTEMP)
        RK4 = 2.33D12*ACID**0.6876*DEXP( - 27.13*GCTEMP)
      END IF
      WATERF = 1./(XMW(1)*SIN1(1))
C

```

```

C      Initialize all variables
C
C0 = SIN1(NCC + 10)*WATERF/162.
G0 = (SIN1(NCC + 11)/162. + SIN1(NCC + 13)/180.)*WATERF
HMFO = SIN1(3)*WATERF
H0 = SIN1(NCC + 15)*WATERF/132.
X0 = SIN1(NCC + 16)*WATERF/150.
F0 = SIN1(4)*WATERF
GLO = SIN1(NCC + 13)*WATERF/180.

C
C      Even though 6 species concern us, there are only 4 independent
C      ODEs. The other 2 species (xylose and glucose) can be found
C      from a material balance
C
Y(1) = C0
Y(2) = HMFO
Y(3) = H0
Y(4) = F0

C
C      X and XEND are the limits of the integration, passed from the
C      input file
C
X = REAL(1)
XEND = REAL(2)
JFLAG = 0
10  CONTINUE
DO 15 I = 1,N
    IF (Y(I).LE.ODO) Y(I) = ODO
15  CONTINUE
CALL GEAR(N,X,XEND,Y,TEST1,TEST2,EPS,NOUT,XOUT,NWS,WS,NA,A,
1    JFLAG,H,NSTEP,IORDER,NDERIV)
IF (JFLAG) 900,910,20
20  GO TO (30,40,10) JFLAG
30  CONTINUE
DO 35 I = 1,N
    IF (Y(I).LE.ODO) Y(I) = ODO
35  CONTINUE

C
C      Evaluate values of the dependent variables (glucose & xylose)
C
G = G0 - (Y(2) - HMFO) - (Y(1) - C0)
XX = X0 - (Y(4) - F0) - (Y(3) - H0)

C
C      Evaluate the reaction rates and derivative values
C
RATE1 = RK1*Y(1)
RATE2 = RK2*G
RATE3 = RK3*Y(3)
RATE4 = RK4*XX
WS(1) = - RATE1
WS(2) = RATE2
WS(3) = - RATE3
WS(4) = RATE4
GO TO 10
40  G = G0 - (Y(2) - HMFO) - (Y(1) - C0)
XX = X0 - (Y(4) - F0) - (Y(3) - H0)
WRITE(NTRMNL,100),X,Y,G,XX

C
C      Store values for results pass
C

```

```

REAL(7*L + 5) = X
REAL(7*L + 6) = G
REAL(7*L + 7) = XX
DO 45 I = 1,4
    J = 7*L + I + 7
    REAL(J) = Y(I)
45  CONTINUE
    L = L + 1
    GO TO 10
900  WRITE(NTRMNL,200),JFLAG
    GO TO 999
910  WRITE(NTRMNL,300)
C
C    Copy inlet stream into outlet stream
C
C    CALL USRCPY(IDS(1,1),1,1,NSIN,NSOUT)
C
C    Copy the results from GEAR into the outlet stream
C
WATERF = 1./WATERF
SOUT1(NCC + 10) = 162.*Y(1)*WATERF
SOUT1(NCC + 11) = 0.
SOUT1(NCC + 13) = 180.*G*WATERF
SOUT1(NCC + 15) = 132.*Y(3)*WATERF
SOUT1(NCC + 16) = 150.*XX*WATERF
SOUT1(3) = Y(2)*WATERF
SOUT1(4) = Y(4)*WATERF
S1 = ODO
S2 = ODO
S3 = ODO
DO 220 I = 1,NCC
    IF (I.EQ.1) GO TO 210
    S2 = S2 + SOUT1(I)*XMW(I)
    S3 = S3 + SOUT1(I)
210  CONTINUE
    S1 = S1 + SIN1(I)*XMW(I)
220  CONTINUE
    SST = S2
    I1 = NCC + 9
    DO 250 I = 1,NNCC
        S1 = S1 + SIN1(I + I1)
        S2 = S2 + SOUT1(I + I1)
250  CONTINUE
    SST = SST + (S1 - S2)
    SOUT1(1) = (S1 - S2)/XMW(1)
    S3 = S3 + SOUT1(1)
    SOUT1(NCC + 9) = SST/S3
    N1 = NCC + 1
    SOUT1(N1) = ODO
    DO 160 I = 1,NCC
        SOUT1(N1) = SOUT1(N1) + SOUT1(I)
160  CONTINUE
    SOUT1(NCC + 2) = TEMP
    SOUT1(NCC + 3) = PRES
    N1 = NCC + 9
    N2 = N1 + NNCC + 1
    SOUT1(N2) = ODO
    DO 170 I = 1,NNCC
        SOUT1(N2) = SOUT1(N2) + SOUT1(N1 + I)
170  CONTINUE

```

```

      SOUT1(N2 + 1) = TEMP
      SOUT1(N2 + 2) = PRES
C
C      Flash the outlet stream to find out energy requirements
C
      CALL FLASH(SOUT1 ,NSUBS ,IDXSUB,ITYPE ,NBOPST,KODE ,NPKODE,
1          KPHASE,MXIT ,ETOL ,TEMP ,PRES ,GUESS ,LMSG ,
2          LPMSG ,IRESTR,KRSLT ,RETN ,IRETN ,LCFLAG)
      IF (LCFLAG.NE.0) WRITE(NTRMNL,950),LCFLAG
      N1 = NCC + NNCC + 9
      SINFO(1) = - ((SOUT1(NCC + 1)*SOUT1(NCC + 9)*SOUT1(NCC + 4) +
1          SOUT1(N1 + 1)*SOUT1(N1 + 4)) - (SIN1(NCC + 1)*
2          SIN1(NCC + 9)*SIN1(NCC + 4) + SIN1(N1 + 1)*
3          SIN1(N1 + 4)))
      GO TO 999
C
C      The following is the report writing section
C
500    CONTINUE
      II = (INT(1) + 1) + 25
      CALL RPTHDR(II,0,3,ISUB)
      WRITE(NRPT,920)
      WRITE(NRPT,930)
      WRITE(NRPT,940), (REAL(J),J=5,7*(INT(1)+1)+4)
100    FORMAT(1X,F6.2,6D11.3)
200    FORMAT(1X,'INTEGRATION HALTED BECAUSE OF ERROR CONDITION 'I3)
300    FORMAT(1X,'INTEGRATION COMPLETED SUCCESSFULLY')
920    FORMAT(/20X,'PROFILES (KGMOL/L) ARE AS FOLLOWS:')
930    FORMAT(3X,'TIME',3X,'GCOSE',6X,'XLOSE',5X,'CCLOSE',7X,
1'HM',6X,'HCOSE',6X,'FURF')
940    FORMAT(1X,F6.2,6D11.3)
950    FORMAT(1X,'FLASH DID NOT CONVERGE. LCFLAG = ',I1)
999    RETURN
      END

```

```

SUBROUTINE USR003(NSIN ,NINFI ,SIN1 ,SIN2 ,SIN3 ,SIN4 ,
1      SINFI ,NSOUT ,NINFO ,SOUT1 ,SOUT2 ,SOUT3 ,SOUT4 ,
2      SINFO ,NSUBS ,IDXSUB,ITYPE ,NINT ,INT ,NREAL ,
3      REAL ,IDS ,NPD ,NBOPST,NIW ,IW ,NW ,
4      W ,NSIZE ,SIZE)
C*****
C      This subroutine is the first version of the ABE fermentor.
C      Currently (8/05/85) it handles only one input and two output
C      streams of stream class MIXEDNC. Some additional requirements*
C      are as follows:
C
C      ** Begin Changes ** 8/27/85
C      Real(15): now used to incorporate butanol inhibition
C      Real(16) - Real(20) are now left available to the user for
C      whatever requirements may crop up.
C      ** End Changes **
C      ** Begin Changes ** 8/28/85
C      N changed from 11 to 2, since other nine variables depend only
C      on the first.
C      yin(11) inserted in dimension statement. Will accommodate the*
C      initial values
C      ** End Changes **
C      (1) The component lists have to be in the following order:
C          CONVENTIONAL: water,sulfuric acid,hmf,furfural,
C                      acetone,butanol,ethanol,acetic acid,
C                      butyric acid,i-propanol,acetoin,carbon*
C                      dioxide,hydrogen,hydrochloric acid.
C          NONCONVEN   : crystalline cellulose,amorphous cellu-
C                      lose,cellebiose,glucose,enzyme,hemi-
C                      cellulose,xylose,lignin,biomass.
C      Additional components may be added to these lists as
C      required.
C      (2) SI units have been used.
C      (3) Int(1)-Int(6): codes for products whose yields have been*
C          supplied. Product codes are:
C
C              Code      Product
C              1          Acetone
C              2          Butanol
C              3          Ethanol
C              4          Acetic acid
C              5          Butyric acid
C              6          Isopropanol
C              7          Acetoin
C              8          C-Dioxide
C              9          Hydrogen
C
C          Int(7)      : no. of records to be retained for results*
C                      pass
C      (4) Real(1)      : lower limit for integration (hr)
C          Real(2)      : upper limit for integration (hr)
C          Real(3)      : temperature of hydrolyzer (K)
C          Real(4)      : pressure of hydrolyzer (Pa)
C          Real(5)-(10) : values for product yields (mol/100 mol
C                      glucose fermented) for 6 the products
C                      specified in int(1)-(6)
C          Real(11)     : % carbon recovery in products
C          Real(12)     : mu-max in Monod growth equation
C          Real(13)     : Ks in Monod growth equation
C          Real(14)     : m, the maintenance coefficient
C      (5) In addition to these 14 spaces for the real vector, space

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C      must be kept to store profiles for the results pass.      *
C      The additional spaces must equal at least 12*(int(7)+1) *
C      in number. *
C      (6) The dimension of RETN has to be 6*NCC + 37 *
C      (7) In the absence of any better method, conversion of xylose *
C      to the products is taken to follow the same yield para- *
C      meters as those estimated for fermentation of glucose. *
C      *
C      See papers by Papoutsakis et al. B & B. 26, 174 (1984) and *
C      B & B. 27, 681 (1985) for a discussion on the overall equation *
C      used to model the fermentation process. *
C      *
C      Subroutines called are: GEAR, RPTHDR, USRCPY, FLASH, DGELG *
C      *
C*****
      IMPLICIT REAL*8(A-H,O-Z)
      REAL EPS2
      CHARACTER LID(12)*12
      DIMENSION SIN1(1) ,SIN2(1) ,SIN3(1) ,SIN4(1) ,
1      SINFI(1) ,SOUT1(1) ,SOUT2(1) ,SOUT3(1) ,
2      SOUT4(1) ,SINFO(1) ,IDXSUB(NSUBS),ITYPE(NSUBS) ,
3      INT(NINT) ,REAL(NREAL),IDS(2,13) ,NBOPST(3,NPO) ,
4      IW(NIW) ,W(NW) ,SIZE(NSIZE) ,WS(187) ,
5      A(11,11) ,XOUT(100) ,Y(11) ,RETN(103) ,
6      IRETN(6) ,AA(11,11) ,B(11) ,BB(11) ,
7      COEFF(10) ,YIELD(9) ,AG(242) ,IVECT(11,9) ,
8      YIN(11)
      COMMON /USER/ RMISS ,IMISS ,NGBAL ,IPASS ,IRESTR ,ICONVG,
1      LMSG ,LPMSG ,KFLAG ,NHSTRY ,NRPT ,NTRMNL,
2      ISIZE
      COMMON /NCOMP/ NCC ,NNCC
      COMMON /IDSCC/ IDSCC(2,1)
      COMMON /IDSNCC/ IDSNCC(2,1)
      COMMON /IDXCC/ IDXCC(1)
      COMMON /IDXNCC/ IDXNCC(1)
      COMMON /MW/ XMW(1)
      COMMON /RPTGLB/ IREPC,L,ISUB(10)

C
C      The next two lines are for GEAR's benefit
C
      COMMON /GEARLC/ XDUMB(70),IDUMB(84)
      DATA N,TEST1,TEST2,EPS1,NWS,NAG/2,1D-10,1D0,,1D0,187,242/
      DATA KODE,NPKODE,KPHASE,MXIT,ETOL,KRSLT/2,2,0,30,1D-4,2/
      DATA EPS2/1E-15/
      DATA IVECT/7*0,1,-1,8*0,1,13*0,1,5*0,1,-1,1,-1,8*0,1,-1,
1      12*0,1,12*0,1,0,1,5*0,1,0,0,2,0,0,1,8*0/
      DATA LID/'BIOMASS','GLUCOSE','ACETONE','BUTANOL','ETHANOL',
1      'ACETIC ACID','BUTYRIC ACID','I-PROPANOL',
2      'ACETOIN','C-DIOXIDE','HYDROGEN','ATP'/
      DATA A/1,2,0D0,2,8*0D0,-1,1,0D0,1,10*0D0,-1,9*0D0,1,-1,
1      8*0D0,-1,10*0D0,-1,-2,9*0D0,-1,-2,9*0D0,-1,11*0D0,
2      -1,9*0D0,-1,-2,8*0D0,-2,9*0D0/

C
C      Go to 600 for Results pass
C
      IF (IPASS.EQ.4) GO TO 600
      L = 0
      NOUT = - INT(7)
      TEMP = REAL(3)
      PRES = REAL(4)

```

```

C
C      Set up the A matrix
C
DO 50 J = 1,11
  DO 50 I = 1,11
    AA(I,J) = A(I,J)
50  CONTINUE
DO 100 I = 1,6
  K = I + 5
  DO 100 J = 1,11
    A(K,J) = IVECT(J,INT(I))
    AA(K,J) = A(K,J)
100 CONTINUE
C
C      Set up the RHS's of the set of simultaneous eqs.
C
B(1) = 200./((100.-REAL(11)) - 2.
B(2) = 0.
B(3) = 0.
B(4) = 1.75
B(5) = 0.
DO 150 I = 1,11
  IF (I.GT.5) THEN
    B(I) = (2.+B(1))*REAL(I - 1)/100.
  END IF
  BB(I) = B(I)
150 CONTINUE
C
C      Solve the set of simultaneous linear equations
C
CALL DGELG(BB,AA,11,1,EPS2,IER)
IF (IER.NE.0) TYPE 900,IER
C
C      Calculate the coefficients of the 9 products & ATP
C      in the overall equation
C
DO 250 I = 1,9
  COEFF(I) = 0D0
  DO 200 K = 1,11
    COEFF(I) = COEFF(I) + IVECT(K,I)*BB(K)
200 CONTINUE
250 CONTINUE
COEFF(10) = 2.*BB(1) - 29.7 + BB(5)
CFGL = 2. + BB(1)
DENOM = 1./((180.*CFGL)
C
C      Evaluate the yields (g/g glucose fermented) of
C      the products
C
DO 300 I = 1,9
  YIELD(I) = XMW(I + 4)*COEFF(I)*DENOM
  IF (YIELD(I).LE.0D0) YIELD(I) = 0D0
300 CONTINUE
YBMASS = 295.08*DENOM
YBMINV = 1D0/YBMASS
C
C      Initialize variables for GEAR and convert inlet
C      flowrates (SI) to concentrations (g/L)
C
T = 1D3/(SIN1(1)*XMW(1))

```

```

      GLUC = SIN1(NCC + 13)
      XYL = SIN1(NCC + 16)
      Y(1) = SIN1(NCC + 18)*T
      Y(2) = (GLUC + XYL)*T
      DO 325 I = 1,11
        IF (I.GE.3) THEN
          I2 = I + 2
          Y(I) = SIN1(I2)*XMW(I2)
        END IF
        YIN(I) = Y(I)
325    CONTINUE
C
C      X and XEND are the limits of the integration, passed from the
C      input file
C
      X = REAL(1)
      XEND = REAL(2)
      JFLAG = 0
350    CALL GEAR(N,X,XEND,Y,TEST1,TEST2,EPS1,NOUT,XOUT,NWS,WS,NAG,AG,
1      JFLAG,H,NSTEP,IORDER,NDERIV)
      IF (JFLAG) 500,550,400
      GO TO (425,450,350) JFLAG
400    C
C      Evaluate the reaction rates and derivative values
C
425    CONTINUE
      DELBMS = YBMINV*(Y(1) - YIN(1))
      DO 430 I = N + 1,11
        Y(I) = YIN(I) + DELBMS*YIELD(I - 2)
430    CONTINUE
      DO 440 I = 1,11
        IF (DABS(Y(I)).LE.1D-6) Y(I) = 0D0
440    CONTINUE
C      BRATE = REAL(12)*Y(1)*Y(2)/(REAL(13) + Y(2) + REAL(15)*Y(4))
      BRATE=(1.-Y(4)/REAL(15))*REAL(12)*Y(1)*Y(2)/(REAL(13)+Y(2))
      WS(1) = BRATE
      WS(2) = - BRATE*YBMINV - REAL(14)*Y(1)
      GO TO 350
450    CONTINUE
C
C      Store values for results pass
C
      DELBMS = YBMINV*(Y(1) - YIN(1))
      DO 460 I = 3,11
        Y(I) = YIN(I) + DELBMS*YIELD(I - 2)
460    CONTINUE
      TYPE *,X,Y
      REAL(12*L + 21) = X
      DO 475 I = 1,11
        J = 12*L + I + 21
        IF (DABS(Y(I)).LE.1D-6) Y(I) = 0D0
        REAL(J) = Y(I)
475    CONTINUE
      L = L + 1
      GO TO 350
500    TYPE 910,JFLAG
      GO TO 999
550    TYPE 920
C
C      Copy inlet stream into outlet streams

```

```

C      CALL USRCPY(IDS(1,1),1,1,NSIN,NSOUT)
C      CALL USRCPY(IDS(1,1),1,2,NSIN,NSOUT)
C
C      Copy the results from GEAR into the first (gaseous)
C      outlet stream
C
      T = 1DO/T
      SOUT1(12) = Y(10)*T/XMW(12)
      SOUT1(13) = Y(11)*T/XMW(13)
      S1 = ODO
      S2 = ODO
      DO 560 I = 1,NCC
        IF (I.LE.11.OR.I.GE.14) SOUT1(I) = ODO
        S1 = S1 + SOUT1(I)
        S2 = S2 + SOUT1(I)*XMW(I)
560    CONTINUE
      SOUT1(NCC + 1) = S1
      SOUT1(NCC + 2) = TEMP
      SOUT1(NCC + 3) = PRES
      SOUT1(NCC + 9) = S2/S1
      N1 = NCC + 9
      DO 570 I = N1 + 1,N1 + NNCC + 1
        SOUT1(I) = ODO
570    CONTINUE
      SOUT1(N1 + NNCC + 2) = TEMP
      SOUT1(N1 + NNCC + 3) = PRES
C
C      Flash the first outlet stream
C
      CALL FLASH(SOUT1,NSUBS,IDXSUB,ITYPE,NBOPST,KODE,NPKODE,
1      KPHASE,MXIT,ETOL,TEMP,PRES,GUESS,LMSG,
2      LPMSG,IRESTR,KRSLT,RETN,IRETN,LCFLAG)
      IF (LCFLAG.NE.0) TYPE 905,LCFLAG
C
C      Copy the results from GEAR into the second outlet stream
C
      S1 = ODO
      S2 = ODO
      DO 580 I = 1, 11
        IF (I.GE.5) SOUT2(I) = T*Y(I - 2)/XMW(I)
        S1 = S1 + SOUT2(I)
        S2 = S2 + SOUT2(I)*XMW(I)
580    CONTINUE
      DO 585 I = 13,NCC
        S1 = S1 + SOUT2(I)
        S2 = S2 + SOUT2(I)*XMW(I)
585    CONTINUE
      SOUT2(NCC + 1) = S1
      SOUT2(NCC + 2) = TEMP
      SOUT2(NCC + 3) = PRES
      SOUT2(NCC + 9) = S2/S1
      N1 = NCC + 13
      FRAC = GLUC/(GLUC + XYL)
      SOUT2(N1) = FRAC*Y(2)*T
      SOUT2(N1 + 3) = (1. - FRAC)*Y(2)*T
      SOUT2(N1 + 5) = Y(1)*T
      S = ODO
      N1 = NCC + 9
      DO 590 I = 1,NNCC

```

```

      S = S + SOUT2(N1 + 1)
590  CONTINUE
      SOUT2(N1 + NNCC + 1) = S
      SOUT2(N1 + NNCC + 2) = TEMP
      SOUT2(N1 + NNCC + 3) = PRES
C
C      Flash the outlet stream and find energy requirements
C
      CALL FLASH(SOUT2, NSUBS, IDXSUB, ITYPE, NBOPST, KODE, NPKODE,
1         KPHASE, MXIT, ETOL, TEMP, PRES, GUESS, LMSG,
2         LPMSG, IRESTR, KRSLT, RETN, IRETN, LCFLAG)
      IF (LCFLAG.NE.0) TYPE 905, LCFLAG
      N1 = NCC + NNCC + 9
      SINFO(1) = - (SOUT1(NCC + 1)*SOUT1(NCC + 9)*SOUT1(NCC + 4) +
1         SOUT2(NCC + 1)*SOUT2(NCC + 9)*SOUT2(NCC + 4) +
2         SOUT2(N1 + 1)*SOUT2(N1 + 4) - (SIN1(NCC + 1)*
3         SIN1(NCC + 9)*SIN1(NCC + 4) + SIN1(N1 + 1)*
4         SIN1(N1 + 4)))
      GO TO 999
C
C      The following is the report writing section
C
600  CONTINUE
      J = (INT(7) + 1)/5
      IF ((5*J).NE.(INT(7) + 1)) J = J + 1
      II = 14*J + 27
      CALL RPTHDR(II, 0, 3, ISUB)
      CBM = 3DO
      CFGM = - CFGL
      WRITE(NRPT, 940), LID(2), CFGM, LID(1), CBM, YBMAS, (LID(1),
1         COEFF(1-2), YIELD(1-2), I = 3, 11), LID(12),
2         COEFF(10))
      WRITE(NRPT, 950)
      DO 700 I = 1, J
          I1 = (I - 1)*60 + 21
          I2 = I1 + 48
          IF (I2.GE.NREAL) I2 = NREAL
          WRITE(NRPT, 960), (REAL(K1), K1 = I1, I2, 12)
          DO 650 K = 1, 9
              I1 = I1 + 1
              I2 = I2 + 1
              IF (I2.GE.NREAL) I2 = NREAL
              WRITE(NRPT, 970), LID(K), (REAL(K2), K2 = I1, I2, 12)
650      CONTINUE
700  CONTINUE
      I1 = 21
      I2 = 12*INT(7) + 21
      DO 750 I = 1, 12
          WRITE(NTRMNL, *), (REAL(J), J=I1, I2, 12)
          I1 = I1 + 1
          I2 = I2 + 1
750  CONTINUE
900  FORMAT(1X, 'WARNING IN DGELG. IER =', I3/)
905  FORMAT(1X, 'FLASH DID NOT CONVERGE. LCFLAG = ', I1)
910  FORMAT(1X, 'INTEGRATION HALTED BECAUSE OF ERROR CONDITION ', I3)
920  FORMAT(1X, 'INTEGRATION COMPLETED SUCCESSFULLY')
930  FORMAT(1X, F6.2, 2X, 11D12.3)
940  FORMAT(1X, 'THE OVERALL FERMENTATION REACTION IS : '//5X,
1'SPECIES', 20X, 'COEFF', 14X, 'YIELD (G/G GLUCOSE)'/5X, A12, 10X,

```

```
2F12.3/10(5X,A12,10X,F12.3,14X,D12.3/),5X,A12,10X,F12.3/)
950  FORMAT(1X,'PROFILES (G/L) ARE AS FOLLOWS: '/')
960  FORMAT(/1X,'TIME',8X,5D12.4/)
970  FORMAT(1X,A12,5D12.4)
999  RETURN
      END
```

```

      SUBROUTINE USR004(NSIN ,NINFI ,SIN1 ,SIN2 ,SIN3 ,SIN4 ,
1          SINFI ,NSOUT ,NINFO ,SOUT1 ,SOUT2 ,SOUT3 ,SOUT4 ,
2          SINFO ,NSUBS ,IDXSUB ,ITYPE ,NINT ,INT ,NREAL ,
3          REAL ,IDS ,NPO ,NBOPST ,NIW ,IW ,NW ,
4          W ,NSIZE ,SIZE)
C*****
C
C      This subroutine is the first version of an continuous steri-
C      lizer. Currently (9/03/85) it handles only one input and one
C      output stream of stream class MIXEDNC, and one output infor-
C      mation stream of class HEAT. Some additional requirements are
C      as follows:
C
C      (1) SI units have been used.
C      (2) Real(1) : preexponential factor, microorganism death*
C                  rate, X 1D-25 (/s)
C          Real(2) : activation energy for death rate (J/kgmol)*
C          Real(3) : temperature of sterilizer (K)
C          Real(4) : pressure of sterilizer (Pa)
C          Real(5) : diameter of sterilizer (m)
C          Real(6) : diffusion coefficient (m**2/s)
C          Real(7) : required sterility level
C          Real(8) : viscosity of fluid (kg/m s)
C          Real(9) : error tolerance
C          Real(10) : number to be subtracted from guesstimate
C                   of the solution of the nonlinear equation *
C      (3) Int(1) : maximum number of iterations for nonlinear*
C                  search
C      (4) The dimension of RETN has to be 6*NCC + 37
C
C      Subroutines called are: USRNLE, USRCPY, FLASH
C
C      Refer to any standard biotechnology textbook for the design
C      equation for continuous sterilizers.
C*****
      IMPLICIT REAL*8(A-H,O-Z)
      REAL EPS
      DIMENSION SIN1(1) ,SIN2(1) ,SIN3(1) ,SIN4(1) ,
1          SINFI(1) ,SOUT1(1) ,SOUT2(1) ,SOUT3(1) ,
2          SOUT4(1) ,SINFO(1) ,IDXSUB(NSUBS),ITYPE(NSUBS) ,
3          INT(NINT) ,REAL(NREAL),IDS(2,13) ,NBOPST(3,NPO) ,
4          IW(NIW) ,W(NW) ,SIZE(NSIZE) ,RETN(103) ,
5          IRETN(6)
      COMMON /USER/ RMISS ,IMISS ,NGBAL ,IPASS ,IRESTR ,ICONVG,
1          LMSG ,LPMSG ,KFLAG ,NHSTRY ,NRPT ,NTRMNL,
2          ISIZE
      COMMON /NCOMP/ NCC ,NNCC
      COMMON /IDSCC/ IDSCC(2,1)
      COMMON /IDSNCC/ IDSNCC(2,1)
      COMMON /IDXCC/ IDXCC(1)
      COMMON /IDXNCC/ IDXNCC(1)
      COMMON /MW/ XMW(1)
      COMMON /RPTGLB/ IREPFL,ISUB(10)
      DATA KODE,NPKODE,KPHASE,MXIT,ETOL,KRSLT/2,2,0,30,1D-4,2/
      DATA PI,GC/3.1415926,8314.3/
C
C      Go to 400 for results pass
C
      IF (IPASS.EQ.4) GO TO 500
      MAXIT = INT(1)

```

```

      EPS = REAL(9)
      TEMP = REAL(3)
      PRES = REAL(4)
      DIA = REAL(5)

C
C      Evaluate fluid velocity, death rate
C
      VFLOW = SIN1(NCC + 1)*SIN1(NCC + 9)/SIN1(NCC + 8) +
1      SIN1(NCC + NNCC + 10)/SIN1(NCC + NNCC + 17)
      VEL = VFLOW/(PI*DIA**2./4.)
      C1 = REAL(2)/(GC*TEMP)
      IF (C1.LE.50.) THEN
        RK = REAL(1)*(DEXP(-C1)*1D25)
      ELSE
        RK = 1928.75*REAL(1)*DEXP(-C1 + 50.)
      END IF
      TYPE *,VEL,RK,DELTA

C
C      Evaluate the Reynolds number & dispersion coefficient
C
      REYNLD = DIA*VEL*SIN1(NCC + 8)/REAL(8)
      IF (REYNLD.LE.2100.) THEN
        DISP = REAL(6) + (VEL*DIA)**2./((192.*REAL(6)))
      ELSE
        FRICTF = 0.0791/(REYNLD**.25)
        DISP = 3.57*VEL*DIA*DSQRT(FRICTF)
      END IF
      DELTA = DSQRT(1. + 4.*RK*DISP/(VEL**2.))
      RSL = REAL(7)

C
C      Evaluate the initial guess to the solution of the nle
C
      XST = DLOG(RSL*((1. + DELTA)**2.)/(4.*DELTA))
      XST = 2.*XST/(1. - DELTA) - REAL(10)

C
C      Solve the nonlinear equation
C
      CALL USRNLE(X,F,DERF,XST,EPS,MAXIT,IER,DELTA,RSL)
      GO TO (40,30,20),IER + 1
20    WRITE(NTRMNL,900),X,F
      TYPE 900,X,F
      GO TO 50
30    WRITE(NTRMNL,910),X,F
      TYPE 910,X,F
      GO TO 50
40    WRITE(NTRMNL,920),X,F
      TYPE 920,X,F
50    CONTINUE

C
C      Calculate the lengths with/without dispersion
C
      RLENG1 = X*DISP/VEL
      RLENG2 = -DLOG(REAL(7))*VEL/RK

C
C      Copy inlet stream into outlet stream
C
      CALL USRCPY(IDS(1,1),1,1,NSIN,NSOUT)
      SOUT1(NCC + 2) = TEMP
      SOUT1(NCC + 3) = PRES
      SOUT1(NCC + NNCC + 11) = TEMP

```

```

      SOUT1(NCC + NNCC + 12) = PRES
C
C      Flash the outlet stream to find energy requirements
C
      CALL FLASH(SOUT1 ,NSUBS ,IDXSUB,ITYPE ,NBOPST,KODE ,NPKODE,
1          KPHASE,MXIT ,ETOL ,TEMP ,PRES ,GUESS ,LMSG ,
2          LPMSG ,IRESTR,KRSLT ,RETN ,IRETN ,LCFLAG)
      IF (LCFLAG.NE.0) WRITE(NTRMNL,950) LCFLAG
      N2 = NCC + NNCC + 9
C
C      Calculate energy requirements
C
      SINFO(1) = - ((SOUT1(NCC + 1)*SOUT1(NCC + 9)*SOUT1(NCC + 4) +
1          SOUT1(N2 + 1)*SOUT1(N2 + 4)) - (SIN1(NCC + 1)*
2          SIN1(NCC + 9)*SIN1(NCC + 4) + SIN1(N2 + 1)*
3          SIN1(N2 + 4)))
      GO TO 999
C
C      The following is the report writing section
C
500      CONTINUE
      WRITE(NRPT,925),(REAL(K),K=1,8)
      WRITE(NRPT,930),RK,VEL,REYNLD,DISP,X,RLENG1,RLENG2
900      FORMAT(1X,'DERIV = 0. X,F VALUES >>','2D14.5)
910      FORMAT(1X,'EXCEEDED MAXIT. X,F VALUES >>','2D14.5)
920      FORMAT(1X,'CONVERGED. X,F VALUES >>','2D14.5)
925      FORMAT(/20X,'KO FOR SPORE DEATH RATE =','5X,D14.5,' /SEC',
1/20X,'DELTA E FOR SPORE DEATH RATE =','D14.5,' J/KGMOL',/20X
2,'TEMPERATURE OF STERILIZER =','3X,D14.5,' K',/20X,'PRESSURE
3 OF STERILIZER =','6X,D14.5,' PA',/20X,'DIAMETER OF STERILIZ
4ER =','6X,D14.5,' M',/20X,'DIFFUSION COEFFICIENT =','7X,D14.5
5,' SQ M/SEC',/20X,'REQUIRED STERILITY LEVEL =','4X,D14.5,/20
6X,'VISCOSITY OF FLUID =','10X,D14.5,' KG/M SEC')
930      FORMAT(/20X,'SPORE DEATH RATE =','12X,D14.5,' PER SEC',/2
10X,'FLUID VELOCITY IN STERILIZER =','D14.5,' M/SEC',/20X,'R
2EYNOLDS NUMBER =','13X,D14.5,/20X,'DISPERSION COEFFICIENT =
3','6X,D14.5,' M**2/S',/20X,'PECLET NUMBER =','15X,D14.5,/20
4X,'LENGTH OF THE STERILIZER =','4X,D14.5,' M WITH DISP'/20X
5,'LENGTH OF THE STERILIZER =','4X,D14.5,' M W/OUT DISP')
940      FORMAT(20X,'DISPERSION CODE =','13X,I2,/20X,'CODE = 1 => D
11SPERSION PRESENT, CODE = 2 IF ABSENT')
950      FORMAT(1X,'FLASH DID NOT CONVERGE. LCFLAG =','I1)
999      RETURN
      END

```

APPENDIX B

Sample Input Data File and Output Report

This appendix contains a sample input data file and output report from an ASPEN simulation. The two files for the acid hydrolysis simulations are presented here; similar files exist for the other sections.

Since most of the components in the simulation are unconventional (e.g. lignin, sugars, etc.), the ASPEN data banks do not contain information on them. Consequently, in the input data file the input values for various parameters such as molecular weights, specific heat coefficients, etc., are defined in the PROP-DATA section. The property streams in the simulation are defined to have two substreams - one MIXED (which is of the same type as the streams in other process simulators), and the other NCPSD. The latter substream is used to represent the flow of nonconventional solids which have the particle size distribution attribute. The remainder of the input data file is similar to data files for other process simulators; if a detailed explanation is required, the interested reader is referred to the ASPEN User Manual. The output report is self-explanatory, and shows the material and energy balances around each unit, and the status of each stream in the flowsheet.

```

NEW
TITLE 'THE ABE PROCESS'
DESCRIPTION 'ACID HYDROLYSIS'
IN-UNITS SI
OUT-UNITS SI
HISTORY MSG-LEVEL STREAMS = 6
PROPERTIES SYSOP4 GLOBAL
COMPONENTS CCLOSE / ACLOSE / CLBOSE / GCOSE / ENZYME / WATER H2O / &
HCLOSE / XYLOSE / LIGNIN / H2SO4 HCL / HMF C5H4O2 / &
FURFURAL C5H4O2
ATTR-COMPS ENZYME CAUSR1 / CCLOSE / ACLOSE / CLBOSE / GCOSE / HCLOSE / &
XYLOSE / LIGNIN
COMP-NAMES CCLOSE CRYSTALLINE-CELLULOSE / ACLOSE AMORPHOUS-CELLULOSE /
CLBOSE CELLOBIOSE / GCOSE GLUCOSE / HCLOSE HEMICELLULOSE
NC-PROPS CCLOSE ENTHALPY ENTHLUSR / DENSITY DNSTYUSR
NC-PROPS ACLOSE ENTHALPY ENTHLUSR / DENSITY DNSTYUSR
NC-PROPS CLBOSE ENTHALPY ENTHLUSR / DENSITY DNSTYUSR
NC-PROPS GCOSE ENTHALPY ENTHLUSR / DENSITY DNSTYUSR
NC-PROPS ENZYME ENTHALPY ENTHLUSR / DENSITY DNSTYUSR
NC-PROPS HCLOSE ENTHALPY ENTHLUSR / DENSITY DNSTYUSR
NC-PROPS XYLOSE ENTHALPY ENTHLUSR / DENSITY DNSTYUSR
NC-PROPS LIGNIN ENTHALPY ENTHLUSR / DENSITY DNSTYUSR
PROP-DATA
PROP-LIST ENTUA / DNSUA
PVAL CCLOSE 85.0 2301.2 0 0 0 / 705.45 0 0 0 0
PVAL ACLOSE 85.0 2301.2 0 0 0 / 705.45 0 0 0 0
PVAL CLBOSE 85.0 2301.2 0 0 0 / 705.45 0 0 0 0
PVAL GCOSE 85.0 2301.2 0 0 0 / 705.45 0 0 0 0
PVAL HCLOSE 85.0 2301.2 0 0 0 / 705.45 0 0 0 0
PVAL XYLOSE 85.0 2301.2 0 0 0 / 705.45 0 0 0 0
PVAL LIGNIN 85.0 2301.2 0 0 0 / 705.45 0 0 0 0
PVAL ENZYME 1.0 0.0 0 0 0 / 1000 0 0 0 0
PROP-LIST DHFORM / DGFORM
PVAL FURFURAL -2.092D8 / -1.255D8
PVAL HMF -2.092D8 / -1.255D8
PROP-LIST MW
PVAL HMF 126.0
PVAL H2SO4 98.08
DEF-STREAMS MIXNCPSD ALL
DEF-SUBS-ATTR PSD PSD
INTERVALS 10
SIZE-LIMITS 0/.0002/.0004/.0006/.0008/.001/&
.002/.003/.01/.02/.05
DEF-STREAMS HEAT QHTR QONCH QACHYD QCOOLR
DEF-STREAMS WORK SHAFT1
FLOWSHEET
BLOCK CRUSHER IN = 1 OUT = 2
BLOCK PUMP1 IN = 2 OUT = 3 SHAFT1
BLOCK SLRYTNK IN = 3 4 OUT = 6
BLOCK ACIDIN IN = 6 7 OUT = 7B
BLOCK HEATER1 IN = 7B OUT = 7C QHTR
BLOCK ACIDHYD IN = 7C OUT = 8 QACHYD
BLOCK FICTSEP IN = 8 OUT = 8A 8B
BLOCK QUENCH IN = 8B OUT = 9 10 QONCH
BLOCK COOLER IN = 10 OUT = 10A QCOOLR
BLOCK CENFUG1 IN = 10A OUT = 11 12
BLOCK CENFUG2 IN = 12 OUT = 13 14
BLOCK CENFUG3 IN = 11 13 OUT = 15
BLOCK C-COLMN IN = 15 OUT = 16 17
STREAM 1

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SUBSTREAM MIXED TEMP = 300.15 PRES = 1.013D5
MASS-FLOW WATER 45.47
SUBSTREAM NCPSD TEMP = 300.15 PRES = 1.013D5
MASS-FLOW LIGNIN 7.88 / HCLOSE 10.71 /%
ACLOSE 7.24 / CCLOSE 19.64
SUBS-ATTR FSD FRAC = 0 0 0 0 0 0 0 0 .5 .5
STREAM 4
SUBSTREAM MIXED TEMP = 826.9415 PRES = 1.4D6
MASS-FLOW WATER 38.95
STREAM 7
SUBSTREAM MIXED TEMP = 759.375 PRES = 1.4D6
MASS-FLOW H2SO4 1.9587
BLOCK CRUSHER CRUSH
PARAM 0.001 0 2
BWI NCPSD 50
BLOCK PUMP1 PUMP
PARAM PRES = 1.4D6 TYPE = 2
BLOCK SLRYTNK MIXER
BLOCK ACIDIN MIXER
BLOCK HEATER1 HEATER
PARAM TEMP = 468.15 PRES = 1.4D6
BLOCK ACIDHYD USER
DESCRIPTION 'ACID HYDROLYZER'
SUBROUTINE USR002 USR002
PARAM NINT = 2 NREAL = 46
INT 5 6
REAL 0.0 0.25 468.15 1.4D6
BLOCK FICTSEP SEP
FRAC SUBS = MIXED STRM = 8A COMP = H2SO4 FRAC = 1.0
BLOCK QUENCH FLASH2
PARAM TEMP = 373.15 PRES = 1.013D5
FRAC NCPSD 0.0
BLOCK COOLER HEATER
PARAM TEMP = 306.15 PRES = 1.013D5
BLOCK CENFUG1 CFUGE
DIAMETER DIA = 1.0 RPS = 100
CAKE-PROPS SPRES = 1D10 MRES = 1D10
RATIOS RL:R = .74 RC:R = .8 H:R = 1.0
BLOCK CENFUG2 SEP
FRAC SUBS=NCPSD STRM=13 COMP=CLBOSE GCOSE ENZYME XYLOSE&
FRAC = 1.0 1.0 1.0 1.0
BLOCK CENFUG3 MIXER
BLOCK C-COLMN SEP
FRAC SUBS = MIXED STRM = 16 COMP = H2SO4 HMF FURFURAL&
FRAC = 1.0 1.0 1.0
STREAM-REPORT
STANDARD OPTIONS = ALL MASS-FLOW

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 THE ABE PROCESS
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FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
2	CRUSHER	PUMP1	3	PUMP1	SLRYTNK
SHAFT1	PUMP1	----	6	SLRYTNK	ACIDIN
7B	ACIDIN	HEATER1	7C	HEATER1	ACIDHYD
QHTR	HEATER1	----	8	ACIDHYD	FICTSEP
QACHYD	ACIDHYD	----	8A	FICTSEP	----
8B	FICTSEP	QUENCH	9	QUENCH	----
10	QUENCH	COOLER	QONCH	QUENCH	----
10A	COOLER	CENFUG1	QCOOLR	COOLER	----
11	CENFUG1	CENFUG3	12	CENFUG1	CENFUG2
13	CENFUG2	CENFUG3	14	CENFUG2	----
15	CENFUG3	C-COLMN	16	C-COLMN	----
17	C-COLMN	----	1	----	CRUSHER
4	----	SLRYTNK	7	----	ACIDIN

FLOWSHEET CONNECTIVITY BY BLOCKS

BLOCK	INLETS	OUTLETS
CRUSHER	1	2
PUMP1	2	3 SHAFT1
SLRYTNK	3 4	6
ACIDIN	6 7	7B
HEATER1	7B	7C QHTR
ACIDHYD	7C	8 QACHYD
FICTSEP	8	8A 8B
QUENCH	8B	9 10 QONCH
COOLER	10	10A QCOOLR
CENFUG1	10A	11 12
CENFUG2	12	13 14
CENFUG3	11 13	15
C-COLMN	15	16 17

COMPUTATIONAL SEQUENCE

SEQUENCE USED WAS:

CRUSHER PUMP1 SLRYTNK ACIDIN HEATER1 ACIDHYD FICTSEP QUENCH COOLER
 CENFUG1 CENFUG2 CENFUG3 C-COLMN

OVERALL FLOWSHEET BALANCE

CONVENTIONAL COMPONENTS (KMOL/SEC)	*** MASS AND ENERGY BALANCE ***		RELATIVE DIFF.
	IN	OUT	
WATER	4.68609	4.60542	0.172165E-01
H2SO4	0.199704E-01	0.199704E-01	0.000000E+00
HMF	0.000000E+00	0.886747E-02	-1.00000
FURFURAL	0.000000E+00	0.800251E-02	-1.00000
SUBTOTAL (KMOL/SEC)	4.70607	4.64226	0.135588E-01
(KG/SEC)	86.3787	86.8115	-0.498507E-02

OVERALL FLOWSHEET BALANCE (CONTINUED)

NON-CONVENTIONAL COMPONENTS (KG/SEC)

CCLOSE	19.6400	17.7014	0.987066E-01
ACLOSE	7.24000	0.000000E+00	1.000000
CLBOSE	0.000000E+00	0.000000E+00	0.000000E+00
GCOSE	0.000000E+00	8.60230	-1.000000
ENZYME	0.000000E+00	0.000000E+00	0.000000E+00
HCLOSE	10.7100	0.854619	0.920204
XYLOSE	0.000000E+00	9.99892	-1.000000
LIGNIN	7.88000	7.88000	-0.281782E-16
SUBTOTAL (KG/SEC)	45.4700	45.0372	0.951752E-02
TOTAL BALANCE			
MASS (KG/SEC)	131.849	131.849	-0.293345E-09
ENTHALPY (WATT)	-0.117860E+10	-0.117864E+10	0.407567E-04

THE ABE PROCESS
UNIT OPERATIONS BLOCK SECTION

CRUSHER (CRUSH): CRUSHER
INLET = 1 OUTLET = 2
PROPERTY OPTION SET SYSOP4

*** MASS AND ENERGY BALANCE ***			
	IN	OUT	RELATIVE DIFF.
CONVENTIONAL COMPONENTS (KMOL/SEC)			
WATER	2.52401	2.52401	0.000000E+00
H2SO4	0.000000E+00	0.000000E+00	0.000000E+00
HMF	0.000000E+00	0.000000E+00	0.000000E+00
FURFURAL	0.000000E+00	0.000000E+00	0.000000E+00
SUBTOTAL (KMOL/SEC)	2.52401	2.52401	0.000000E+00
(KG/SEC)	45.4700	45.4700	0.000000E+00
NON-CONVENTIONAL COMPONENTS (KG/SEC)			
CCLOSE	19.6400	19.6400	-0.226115E-16
ACLOSE	7.24000	7.24000	-0.306691E-16
CLBOSE	0.000000E+00	0.000000E+00	0.000000E+00
GCOSE	0.000000E+00	0.000000E+00	0.000000E+00
ENZYME	0.000000E+00	0.000000E+00	0.000000E+00
HCLOSE	10.7100	10.7100	-0.207325E-16
XYLOSE	0.000000E+00	0.000000E+00	0.000000E+00
LIGNIN	7.88000	7.88000	-0.281782E-16
SUBTOTAL (KG/SEC)	45.4700	45.4700	-0.195333E-16
TOTAL BALANCE			
MASS (KG/SEC)	90.9400	90.9400	0.000000E+00
ENTHALPY (WATT)	-0.694385E+09	-0.694385E+09	-0.214595E-16

*** INPUT DATA ***

OPERATING MODE: 0 = PRIMARY, 1 = SECONDARY	0
CRUSHER TYPE: 1 = GYRATORY/JAW, 2 = SINGLE ROLL	
3 = MULTIPLE ROLL, 4 = CAGE MILL	2
DIAMETER OF SOLIDS OUTLET ,METER	0.00100000
BOND WORK INDEX FOR SUBSTREAM NCPSD	50.0000

*** RESULTS ***

POWER REQUIREMENT ,WATT	881.439
PARTICLE DIAMETER WHICH IS	
LARGER THAN 80% OF INLET MASS METER	0.038000
PARTICLE DIAMETER WHICH IS	
LARGER THAN 80% OF OUTLET MASS METER	0.00086186

PUMP (PUMP): PUMP1
INLET = 2 OUTLET = 3
PROPERTY OPTION SET SYSOP4

PUMP (PUMP): PUMP1 (CONTINUED)

*** MASS AND ENERGY BALANCE ***			
	IN	OUT	RELATIVE DIFF.
CONVENTIONAL COMPONENTS (KMOL/SEC)			
WATER	2.52401	2.52401	0.000000E+00
H2SO4	0.000000E+00	0.000000E+00	0.000000E+00
HMF	0.000000E+00	0.000000E+00	0.000000E+00
FURFURAL	0.000000E+00	0.000000E+00	0.000000E+00
SUBTOTAL (KMOL/SEC)	2.52401	2.52401	0.000000E+00
(KG/SEC)	45.4700	45.4700	0.000000E+00
NON-CONVENTIONAL COMPONENTS (KG/SEC)			
CCLOSE	19.6400	19.6400	0.000000E+00
ACLOSE	7.24000	7.24000	0.000000E+00
CLBOSE	0.000000E+00	0.000000E+00	0.000000E+00
GCOSE	0.000000E+00	0.000000E+00	0.000000E+00
ENZYME	0.000000E+00	0.000000E+00	0.000000E+00
HCLOSE	10.7100	10.7100	0.000000E+00
XYLOSE	0.000000E+00	0.000000E+00	0.000000E+00
LIGNIN	7.88000	7.88000	0.000000E+00
SUBTOTAL (KG/SEC)	45.4700	45.4700	0.000000E+00
TOTAL BALANCE			
MASS (KG/SEC)	90.9400	90.9400	0.000000E+00
ENTHALPY (WATT)	-0.694385E+09	-0.694385E+09	0.695742E-08

*** INPUT DATA ***

TYPE OF PUMP: 1=CENTRIFUGAL PUMP;
 2, SLURRY PUMP; 3, POSITIVE DISPLACEMENT PUMP 2
 REQUIRED EXIT PRESSURE ,N/SQM 1,400,000.
 PUMP EFFICIENCY , MISSING
 DRIVER EFFICIENCY , 1.00000
 SOLID FLOW RATE ,KG/SEC MISSING

*** RESULTS ***

TYPE OF PUMP, (CAL) 2
 VOLUMETRIC FLOW RATE CUM/SEC 0.053706
 DELTA PRESSURE N/SQM 1,298,700.
 FLUID POWER REQUIREMENTWATT 69,748.6
 BRAKE POWER REQUIREMENTWATT 107,305.
 ELECTRICITY REQUIREMENT WATT 107,305.
 PUMP EFFICIENCY (CAL) 0.65000

MIXER (MIXER): SLRYTNK
 INLET STREAM(S): 3 4
 OUTLET STREAM: 6
 PROPERTY OPTION SET SYSOP4

MIXER (MIXER): SLRYTNK (CONTINUED)

*** MASS AND ENERGY BALANCE ***			
	IN	OUT	RELATIVE DIFF.
CONVENTIONAL COMPONENTS (KMOL/SEC)			
WATER	4.68609	4.68609	0.000000E+00
H2SO4	0.000000E+00	0.000000E+00	0.000000E+00
HMF	0.000000E+00	0.000000E+00	0.000000E+00
FURFURAL	0.000000E+00	0.000000E+00	0.000000E+00
SUBTOTAL (KMOL/SEC)	4.68609	4.68609	0.000000E+00
(KG/SEC)	84.4200	84.4200	0.000000E+00
NON-CONVENTIONAL COMPONENTS (KG/SEC)			
CCLOSE	19.6400	19.6400	0.000000E+00
ACLOSE	7.24000	7.24000	0.000000E+00
CLBOSE	0.000000E+00	0.000000E+00	0.000000E+00
GCOSE	0.000000E+00	0.000000E+00	0.000000E+00
ENZYME	0.000000E+00	0.000000E+00	0.000000E+00
HCLOSE	10.7100	10.7100	0.000000E+00
XYLOSE	0.000000E+00	0.000000E+00	0.000000E+00
LIGNIN	7.88000	7.88000	0.000000E+00
SUBTOTAL (KG/SEC)	45.4700	45.4700	0.000000E+00
TOTAL BALANCE			
MASS (KG/SEC)	129.890	129.890	0.000000E+00
ENTHALPY (WATT)	-0.117691E+10	-0.117692E+10	0.197368E-05

*** INPUT DATA ***
 OUTLET PRESSURE ,N/SQM MISSING
 TYPE OF FLASH - TWO PHASE
 MAXIMUM NUMBER OF ITERATIONS IN FLASH 30
 CONVERGENCE TOLERANCE FOR FLASH 0.000100000

MIXER (MIXER): ACIDIN
 INLET STREAM(S): 6 7
 OUTLET STREAM: 7B
 PROPERTY OPTION SET SYSOP4

*** MASS AND ENERGY BALANCE ***			
	IN	OUT	RELATIVE DIFF.
CONVENTIONAL COMPONENTS (KMOL/SEC)			
WATER	4.68609	4.68609	0.000000E+00
H2SO4	0.199704E-01	0.199704E-01	0.000000E+00
HMF	0.000000E+00	0.000000E+00	0.000000E+00
FURFURAL	0.000000E+00	0.000000E+00	0.000000E+00
SUBTOTAL (KMOL/SEC)	4.70607	4.70607	0.000000E+00
(KG/SEC)	86.3787	86.3787	0.000000E+00

THE ABE PROCESS
UNIT OPERATIONS BLOCK SECTION

MIXER (MIXER): ACIDIN (CONTINUED)

NON-CONVENTIONAL COMPONENTS (KG/SEC)

CCLOSE	19.6400	19.6400	0.000000E+00
ACLOSE	7.24000	7.24000	0.000000E+00
CLBOSE	0.000000E+00	0.000000E+00	0.000000E+00
GCOSE	0.000000E+00	0.000000E+00	0.000000E+00
ENZYME	0.000000E+00	0.000000E+00	0.000000E+00
HCLOSE	10.7100	10.7100	0.000000E+00
XYLOSE	0.000000E+00	0.000000E+00	0.000000E+00
LIGNIN	7.88000	7.88000	0.000000E+00
SUBTOTAL (KG/SEC)	45.4700	45.4700	0.000000E+00
TOTAL BALANCE			
MASS (KG/SEC)	131.849	131.849	0.000000E+00
ENTHALPY (WATT)	-0.117849E+10	-0.117849E+10	-0.132360E-07

*** INPUT DATA ***

OUTLET PRESSURE ,N/SQM	MISSING
TYPE OF FLASH - TWO PHASE	
MAXIMUM NUMBER OF ITERATIONS IN FLASH	30
CONVERGENCE TOLERANCE FOR FLASH	0.000100000

GENERAL-HEAT (HEATER): HEATER1

INPUT STREAM: 7B
OUTPUT STREAM: 7C QHTR
PROPERTY OPTION SET SYSOP4

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
CONVENTIONAL COMPONENTS (KMOL/SEC)			
WATER	4.68609	4.68609	0.000000E+00
H2SO4	0.199704E-01	0.199704E-01	0.000000E+00
HMF	0.000000E+00	0.000000E+00	0.000000E+00
FURFURAL	0.000000E+00	0.000000E+00	0.000000E+00
SUBTOTAL (KMOL/SEC)	4.70607	4.70607	0.000000E+00
(KG/SEC)	86.3787	86.3787	0.000000E+00
NON-CONVENTIONAL COMPONENTS (KG/SEC)			
CCLOSE	19.6400	19.6400	0.000000E+00
ACLOSE	7.24000	7.24000	0.000000E+00
CLBOSE	0.000000E+00	0.000000E+00	0.000000E+00
GCOSE	0.000000E+00	0.000000E+00	0.000000E+00
ENZYME	0.000000E+00	0.000000E+00	0.000000E+00
HCLOSE	10.7100	10.7100	0.000000E+00
XYLOSE	0.000000E+00	0.000000E+00	0.000000E+00
LIGNIN	7.88000	7.88000	0.000000E+00
SUBTOTAL (KG/SEC)	45.4700	45.4700	0.000000E+00
TOTAL BALANCE			
MASS (KG/SEC)	131.849	131.849	0.000000E+00
ENTHALPY (WATT)	-0.117849E+10	-0.117849E+10	0.252886E-16

GENERAL-HEAT (HEATER): HEATER1 (CONTINUED)

*** INPUT DATA ***

TWO PHASE TP FLASH
 SPECIFIED TEMPERATURE K 468.15
 SPECIFIED PRESSURE N/SQM 0.14000E+07
 MAXIMUM ITERATION NO. 30
 CONVERGENCE TOLERANCE 0.10000E-03
 TP FLASH, NO INITIAL GUESSES ARE REQUIRED.

*** RESULTS ***

OUTPUT TEMPERATURE K 468.15
 OUTPUT PRESSURE N/SQM 0.14000E+07
 HEAT DUTY WATT 0.11547E+09
 VAPOR FRACTION 1.0000

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
WATER	0.99576	0.99997	0.99576	0.99831
H2SO4	0.42436E-02	0.25775E-04	0.42436E-02	165.06

USER-MODEL (USER): ACIDHYD
 ACID HYDROLYZER
 INPUT STREAMS 7C
 OUTPUT STREAMS 8 QACHYD
 PROPERTY OPTION SET SYSOP4

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
CONVENTIONAL COMPONENTS (KMOL/SEC)			
WATER	4.68609	4.60542	0.172165E-01
H2SO4	0.199704E-01	0.199704E-01	0.000000E+00
HMF	0.000000E+00	0.886747E-02	-1.00000
FURFURAL	0.000000E+00	0.800251E-02	-1.00000
SUBTOTAL (KMOL/SEC)	4.70607	4.64226	0.135588E-01
(KG/SEC)	86.3787	86.8115	-0.498507E-02
NON-CONVENTIONAL COMPONENTS (KG/SEC)			
CCLOSE	19.6400	17.7014	0.987066E-01
ACLOSE	7.24000	0.000000E+00	1.00000
CLBOSE	0.000000E+00	0.000000E+00	0.000000E+00
GCOSE	0.000000E+00	8.60230	-1.00000
ENZYME	0.000000E+00	0.000000E+00	0.000000E+00
HCLOSE	10.7100	0.854619	0.920204
XYLOSE	0.000000E+00	9.99892	-1.00000
LIGNIN	7.88000	7.88000	0.000000E+00
SUBTOTAL (KG/SEC)	45.4700	45.0372	0.951752E-02
TOTAL BALANCE			
MASS (KG/SEC)	131.849	131.849	0.000000E+00
ENTHALPY (WATT)	-0.106302E+10	-0.106302E+10	0.000000E+00

USER-MODEL (USER): ACIDHYD (CONTINUED)

PROFILES (KGMOL/L) ARE AS FOLLOWS:

TIME	GCOSE	XLOSE	CCLOSE	HMF	HCLOSE	FURF
0.00	0.529D-03	0.000D+00	0.144D-02	0.000D+00	0.961D-03	0.000D+00
0.05	0.539D-03	0.374D-03	0.141D-02	0.204D-04	0.580D-03	0.676D-05
0.10	0.547D-03	0.588D-03	0.138D-02	0.412D-04	0.350D-03	0.230D-04
0.15	0.554D-03	0.705D-03	0.135D-02	0.622D-04	0.211D-03	0.446D-04
0.20	0.560D-03	0.765D-03	0.132D-02	0.835D-04	0.128D-03	0.690D-04
0.25	0.566D-03	0.790D-03	0.129D-02	0.105D-03	0.767D-04	0.948D-04

SEPARATOR (SEP): FICTSEP
 INPUT STREAM - 8
 OUTPUT STREAMS - 8A
 8B
 PROPERTY OPTION SET SYSOP4

	*** MASS AND ENERGY BALANCE ***		
	IN	OUT	RELATIVE DIFF.
CONVENTIONAL COMPONENTS (KMOL/SEC)			
WATER	4.60542	4.60542	0.000000E+00
H2SO4	0.199704E-01	0.199704E-01	0.000000E+00
HMF	0.886747E-02	0.886747E-02	0.000000E+00
FURFURAL	0.800251E-02	0.800251E-02	0.000000E+00

SEPARATOR (SEP): FICTSEP (CONTINUED)

NON-CONVENTIONAL COMPONENTS (KG/SEC)

CCLOSE	17.7014	17.7014	0.000000E+00
ACLOSE	0.000000E+00	0.000000E+00	0.000000E+00
CLBOSE	0.000000E+00	0.000000E+00	0.000000E+00
GCOSE	8.60230	8.60230	0.000000E+00
ENZYME	0.000000E+00	0.000000E+00	0.000000E+00
HCLOSE	0.854619	0.854619	0.000000E+00
XYLOSE	9.99892	9.99892	0.000000E+00
LIGNIN	7.88000	7.88000	0.000000E+00
TOTAL BALANCE			
MASS(KG/SEC)	131.849	131.849	0.000000E+00
ENTHALPY(WATT)	-0.104762E+10	-0.104763E+10	0.242617E-05

*** INPUT DATA ***

FLASH SPECS FOR STREAM 8A

TEMPERATURE (K)	MISSING
PRESSURE (N/SQM)	MISSING
VAPOR FRACTION	MISSING
PHASE CODE	2
TEMP ESTIMATE (K)	MISSING
PRES ESTIMATE (N/SQM)	MISSING
MAX. NO. ITERATIONS	25
CONVERGENCE TOL.	0.000100000

FLASH SPECS FOR STREAM 8B

TEMPERATURE (K)	MISSING
PRESSURE (N/SQM)	MISSING
VAPOR FRACTION	MISSING
PHASE CODE	2
TEMP ESTIMATE (K)	MISSING
PRES ESTIMATE (N/SQM)	MISSING
MAX. NO. ITERATIONS	25
CONVERGENCE TOL.	0.000100000

FRACTION OF FEED

SUBSTREAM= MIXED			
STREAM= 8A	CPT= H2SO4	FRACTION=	1.00000

*** RESULTS ***

HEAT DUTY(WATT)	2.541.72
------------------	----------

SEPARATOR (SEP): FICTSEP (CONTINUED)

COMPONENT = WATER		
STREAM	SUBSTREAM	SPLIT FRACTION
8B	MIXED	1.00000

COMPONENT = H2SO4		
STREAM	SUBSTREAM	SPLIT FRACTION
8A	MIXED	1.00000

COMPONENT = HMF		
STREAM	SUBSTREAM	SPLIT FRACTION
8B	MIXED	1.00000

COMPONENT = FURFURAL		
STREAM	SUBSTREAM	SPLIT FRACTION
8B	MIXED	1.00000

COMPONENT = CCLOSE		
STREAM	SUBSTREAM	SPLIT FRACTION
8B	NCPSD	1.00000

COMPONENT = ACLOSE		
STREAM	SUBSTREAM	SPLIT FRACTION

COMPONENT = CLBOSE		
STREAM	SUBSTREAM	SPLIT FRACTION

SEPARATOR (SEP): FICTSEP (CONTINUED)

COMPONENT = GCOSE
 STREAM SUBSTREAM SPLIT FRACTION
 8B NCPSD 1.00000

COMPONENT = ENZYME
 STREAM SUBSTREAM SPLIT FRACTION

COMPONENT = HCLOSE
 STREAM SUBSTREAM SPLIT FRACTION
 8B NCPSD 1.00000

COMPONENT = XYLOSE
 STREAM SUBSTREAM SPLIT FRACTION
 8B NCPSD 1.00000

COMPONENT = LIGNIN
 STREAM SUBSTREAM SPLIT FRACTION
 8B NCPSD 1.00000

FLASH:2-OUTL (FLASH2): QUENCH

INPUT STREAM(S): 8B

OUTPUT STREAM(S): 9 10 QQNCH

PROPERTY OPTION SET SYSOP4

*** MASS AND ENERGY BALANCE ***
 IN OUT

CONVENTIONAL COMPONENTS (KMOL/SEC)	IN	OUT	RELATIVE DIFF.
WATER	4.60542	4.60542	0.875404E-10
H2SO4	0.000000E+00	0.000000E+00	0.000000E+00
HMF	0.886747E-02	0.886747E-02	-0.244441E-07
FURFURAL	0.800251E-02	0.800251E-02	-0.244441E-07
SUBTOTAL (KMOL/SEC)	4.62229	4.62229	0.240189E-16
(KG/SEC)	84.8528	84.8528	-0.455814E-09

FLASH:2-OUTL (FLASH2): QUENCH (CONTINUED)

NON-CONVENTIONAL COMPONENTS (KG/SEC)			
CCLOSE	17.7014	17.7014	0.000000E+00
ACLOSE	0.000000E+00	0.000000E+00	0.000000E+00
CLBOSE	0.000000E+00	0.000000E+00	0.000000E+00
GCOSE	8.60230	8.60230	0.000000E+00
ENZYME	0.000000E+00	0.000000E+00	0.000000E+00
HCLOSE	0.854619	0.854619	0.000000E+00
XYLOSE	9.99892	9.99892	0.000000E+00
LIGNIN	7.88000	7.88000	0.000000E+00
SUBTOTAL (KG/SEC)	45.0372	45.0372	0.000000E+00
TOTAL BALANCE			
MASS (KG/SEC)	129.890	129.890	-0.297768E-09
ENTHALPY (WATT)	-0.104587E+10	-0.104587E+10	-0.569903E-16

*** INPUT DATA ***

TWO PHASE TP FLASH
 SPECIFIED TEMPERATURE K 373.15
 SPECIFIED PRESSURE N/SQM 0.10130E+06
 MAXIMUM ITERATION NO. 30
 CONVERGENCE TOLERANCE 0.10000E-03
 TP FLASH, NO INITIAL GUESSES ARE REQUIRED.
 LIQUID ENTRAINMENT 0.00000E+00
 SOLID SPLIT FRACTIONS:
 SUBSTREAM NO. = 1 MIXED SUBSTREAM, NO SOLID SPLITS.
 SUBSTREAM NO. = 2 VAPOR: 0.00000E+00 LIQUID: 0.10000E+31

*** RESULTS ***

OUTPUT TEMPERATURE K 373.15
 OUTPUT PRESSURE N/SQM 0.10130E+06
 HEAT DUTY WATT -0.20338E+09
 VAPOR FRACTION 0.66936E-01

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
WATER	0.99635	0.99982	0.94799	0.94816
HMF	0.19184E-02	0.94794E-04	0.27339E-01	288.39
FURFURAL	0.17313E-02	0.85348E-04	0.24672E-01	288.39

GENERAL-HEAT (HEATER): COOLER
 INPUT STREAM: 10
 OUTPUT STREAM: 10A QCOOLR
 PROPERTY OPTION SET SYSOP4

GENERAL-HEAT (HEATER): COOLER (CONTINUED)

*** MASS AND ENERGY BALANCE ***			
	IN	OUT	RELATIVE DIFF.
CONVENTIONAL COMPONENTS (KMOL/SEC)			
WATER	4.31211	4.31211	0.000000E+00
H2SO4	0.000000E+00	0.000000E+00	0.000000E+00
HMF	0.408837E-03	0.408837E-03	0.000000E+00
FURFURAL	0.368957E-03	0.368957E-03	0.000000E+00
SUBTOTAL (KMOL/SEC)	4.31289	4.31289	0.000000E+00
(KG/SEC)	77.7697	77.7697	0.000000E+00
NON-CONVENTIONAL COMPONENTS (KG/SEC)			
CCLOSE	17.7014	17.7014	0.000000E+00
ACLOSE	0.000000E+00	0.000000E+00	0.000000E+00
CLBOSE	0.000000E+00	0.000000E+00	0.000000E+00
GCOSE	8.60230	8.60230	0.000000E+00
ENZYME	0.000000E+00	0.000000E+00	0.000000E+00
HCLOSE	0.854619	0.854619	0.000000E+00
XYLOSE	9.99892	9.99892	0.000000E+00
LIGNIN	7.88000	7.88000	0.000000E+00
SUBTOTAL (KG/SEC)	45.0372	45.0372	0.000000E+00
TOTAL BALANCE			
MASS (KG/SEC)	122.807	122.807	0.000000E+00
ENTHALPY (WATT)	-0.117575E+10	-0.117575E+10	0.000000E+00

*** INPUT DATA ***

TWO PHASE TP FLASH
 SPECIFIED TEMPERATURE K 306.15
 SPECIFIED PRESSURE N/SQM 0.10130E+06
 MAXIMUM ITERATION NO. 30
 CONVERGENCE TOLERANCE 0.10000E-03
 TP FLASH, NO INITIAL GUESSES ARE REQUIRED.

*** RESULTS ***

OUTPUT TEMPERATURE K 306.15
 OUTPUT PRESSURE N/SQM 0.10130E+06
 HEAT DUTY WATT -0.30551E+08
 VAPOR FRACTION 0.00000E+00

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
WATER	0.99982	0.99982	0.33780	0.42790E-01
HMF	0.94794E-04	0.94794E-04	0.34808	465.05
FURFURAL	0.85548E-04	0.85548E-04	0.31412	465.05

CENTRIFUGE (CFUGE): CENFUG1
 INLET = 10A OUTLET = 11 12
 PROPERTY OPTION SET SYSOP4

CENTRIFUGE (CFUGE): CENFUG1 (CONTINUED)

*** MASS AND ENERGY BALANCE ***			
	IN	OUT	RELATIVE DIFF.
CONVENTIONAL COMPONENTS (KMOL/SEC)			
WATER	4.31211	4.31211	0.000000E+00
H2SO4	0.000000E+00	0.000000E+00	0.000000E+00
HMF	0.408837E-03	0.408837E-03	0.000000E+00
FURFURAL	0.368957E-03	0.368957E-03	0.000000E+00
SUBTOTAL (KMOL/SEC)	4.31289	4.31289	0.000000E+00
(KG/SEC)	77.7697	77.7697	-0.228413E-16
NON-CONVENTIONAL COMPONENTS (KG/SEC)			
CCLOSE	17.7014	17.7014	0.000000E+00
ACLOSE	0.000000E+00	0.000000E+00	0.000000E+00
CLBOSE	0.000000E+00	0.000000E+00	0.000000E+00
GCOSE	8.60230	8.60230	0.000000E+00
ENZYME	0.000000E+00	0.000000E+00	0.000000E+00
HCLOSE	0.854619	0.854619	0.000000E+00
XYLOSE	9.99892	9.99892	0.000000E+00
LIGNIN	7.88000	7.88000	0.000000E+00
SUBTOTAL (KG/SEC)	45.0372	45.0372	0.000000E+00
TOTAL BALANCE			
MASS (KG/SEC)	122.807	122.807	-0.144646E-16
ENTHALPY (WATT)	-0.120630E+10	-0.120630E+10	0.247055E-16

*** INPUT DATA ***

RATIO RADIUS OF LIQ TO RADIUS OF BOW ,	0.74000
RATIO-RADIUS OF CAKE TO RADIUS OF BOW ,	0.80000
RATIO OF HEIGHT TO RADIUS OF BOW ,	1.00000
CAKE RESISTANCE ,	0.100000+11
FILTER MEDIUM RESISTANCE ,	0.100000+11
MOISTURE CONTENT ,	MISSING
POROSITY OF CAKE ,	0.45000
PARTICLE SPHERICITY ,	0.75000
AVERAGE PARTICLE DIAMETER ,METER	MISSING
SURFACE TENSION ,N/M	0.096065
AVERAGE SOLID DENSITY ,KG/CUM	705.450
DRY SOLIDS FEED MASS FLOW RATE ,KG/SEC	45.0372

*** RESULTS ***

CALCULATED PARTICLE DIAMETER ,METER	0.00081084
RESULTED MOISTURE CONTENT ,	0.0025968
SELECTED BOW RADIUS ,	1.00000
REVOLUTIONS PER SECOND ,HZ	100.000
BASKET HEIGHT ,METER	1.00000

SEPARATOR (SEP): CENFUG2
 INPUT STREAM - 12
 OUTPUT STREAMS - 13
 14
 PROPERTY OPTION SET SYSOP4

SEPARATOR (SEP): CENFUG2 (CONTINUED)

*** MASS AND ENERGY BALANCE ***			
	IN	OUT	RELATIVE DIFF.
CONVENTIONAL COMPONENTS (KMOL/SEC)			
WATER	0.648464E-02	0.648464E-02	0.000000E+00
H2SO4	0.000000E+00	0.000000E+00	0.000000E+00
HMF	0.614817E-06	0.614817E-06	0.000000E+00
FURFURAL	0.554846E-06	0.554846E-06	0.000000E+00
NON-CONVENTIONAL COMPONENTS (KG/SEC)			
CCLOSE	17.7014	17.7014	0.000000E+00
ACLOSE	0.000000E+00	0.000000E+00	0.000000E+00
CLBOSE	0.000000E+00	0.000000E+00	0.000000E+00
GCOSE	8.60230	8.60230	0.000000E+00
ENZYME	0.000000E+00	0.000000E+00	0.000000E+00
HCLOSE	0.854619	0.854619	0.000000E+00
XYLOSE	9.99892	9.99892	0.000000E+00
LIGNIN	7.88000	7.88000	0.000000E+00
TOTAL BALANCE			
MASS (KG/SEC)	45.1542	45.1542	0.000000E+00
ENTHALPY (WATT)	0.298713E+08	0.298713E+08	-0.623556E-16

*** INPUT DATA ***

FLASH SPECS FOR STREAM 13
 TEMPERATURE (K) MISSING
 PRESSURE (N/SQM) MISSING
 VAPOR FRACTION MISSING
 PHASE CODE 2
 TEMP ESTIMATE (K) MISSING
 PRES ESTIMATE (N/SQM) MISSING
 MAX. NO. ITERATIONS 25
 CONVERGENCE TOL. 0.000100000

FLASH SPECS FOR STREAM 14
 TEMPERATURE (K) MISSING
 PRESSURE (N/SQM) MISSING
 VAPOR FRACTION MISSING
 PHASE CODE 2
 TEMP ESTIMATE (K) MISSING
 PRES ESTIMATE (N/SQM) MISSING
 MAX. NO. ITERATIONS 25
 CONVERGENCE TOL. 0.000100000

SEPARATOR (SEP): CENFUG2 (CONTINUED)

FRACTION OF FEED
 SUBSTREAM= NCPSD
 STREAM= 13

CPT= CLBOSE	FRACTION=	1.00000
GCLOSE		1.00000
ENZYME		1.00000
XYLOSE		1.00000

HEAT DUTY(WATT)

*** RESULTS ***
 -0.186265-08

COMPONENT = WATER		
STREAM	SUBSTREAM	SPLIT FRACTION
14	MIXED	1.00000

COMPONENT = H2SO4		
STREAM	SUBSTREAM	SPLIT FRACTION

COMPONENT = HMF		
STREAM	SUBSTREAM	SPLIT FRACTION
14	MIXED	1.00000

COMPONENT = FURFURAL		
STREAM	SUBSTREAM	SPLIT FRACTION
14	MIXED	1.00000

COMPONENT = CCLOSE		
STREAM	SUBSTREAM	SPLIT FRACTION
14	NCPSD	1.00000

COMPONENT = ACLOSE		
STREAM	SUBSTREAM	SPLIT FRACTION

SEPARATOR (SEP): CENFUG2 (CONTINUED)

COMPONENT =	CLBOSE		
STREAM	SUBSTREAM	SPLIT FRACTION	
COMPONENT =	GCOSE		
STREAM	SUBSTREAM	SPLIT FRACTION	
13	NCPSD	1.00000	
COMPONENT =	ENZYME		
STREAM	SUBSTREAM	SPLIT FRACTION	
COMPONENT =	HCLOSE		
STREAM	SUBSTREAM	SPLIT FRACTION	
14	NCPSD	1.00000	
COMPONENT =	XYLOSE		
STREAM	SUBSTREAM	SPLIT FRACTION	
13	NCPSD	1.00000	
COMPONENT =	LIGNIN		
STREAM	SUBSTREAM	SPLIT FRACTION .	
14	NCPSD	1.00000	

MIXER (MIXER): CENFUG3
 INLET STREAM(S): 11 13
 OUTLET STREAM: 15
 PROPERTY OPTION SET SYSOP4

THE ABE PROCESS
UNIT OPERATIONS BLOCK SECTION

MIXER (MIXER): CENFUG3 (CONTINUED)

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*** MASS AND ENERGY BALANCE ***
      IN                               OUT          RELATIVE DIFF.
CONVENTIONAL COMPONENTS (KMOL/SEC)
WATER                4.30563            4.30563            0.000000E+00
H2SO4                0.000000E+00        0.000000E+00        0.000000E+00
HMF                 0.408222E-03        0.408222E-03        0.000000E+00
FURFURAL            0.368402E-03        0.368402E-03        0.000000E+00
SUBTOTAL (KMOL/SEC)  4.30640            4.30640            0.000000E+00
      (KG/SEC )      77.6527            77.6527            0.000000E+00
NON-CONVENTIONAL COMPONENTS (KG/SEC )
CCLOSE              0.000000E+00        0.000000E+00        0.000000E+00
ACLOSE              0.000000E+00        0.000000E+00        0.000000E+00
CLBOSE              0.000000E+00        0.000000E+00        0.000000E+00
GCLOSE              8.60230            8.60230            0.000000E+00
ENZYME              0.000000E+00        0.000000E+00        0.000000E+00
HCLOSE              0.000000E+00        0.000000E+00        0.000000E+00
XYLOSE              9.99892            9.99892            0.000000E+00
LIGNIN              0.000000E+00        0.000000E+00        0.000000E+00
SUBTOTAL (KG/SEC )  18.6012            18.6012            0.000000E+00
TOTAL BALANCE
MASS (KG/SEC )      96.2539            96.2539            0.000000E+00
ENTHALPY (WATT )    -0.122307E+10        -0.122307E+10        -0.341137E-15

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*** INPUT DATA ***
OUTLET PRESSURE ,N/SQM                MISSING
TYPE OF FLASH - TWO PHASE
MAXIMUM NUMBER OF ITERATIONS IN FLASH                30
CONVERGENCE TOLERANCE FOR FLASH                0.000100000

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SEPARATOR (SEP ): C-COLMN
INPUT STREAM - 15
OUTPUT STREAMS - 16
                  17
PROPERTY OPTION SET SYSOP4

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*** MASS AND ENERGY BALANCE ***
      IN                               OUT          RELATIVE DIFF.
CONVENTIONAL COMPONENTS (KMOL/SEC)
WATER                4.30563            4.30563            0.000000E+00
H2SO4                0.000000E+00        0.000000E+00        0.000000E+00
HMF                 0.408222E-03        0.408222E-03        0.000000E+00
FURFURAL            0.368402E-03        0.368402E-03        0.000000E+00

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SEPARATOR (SEP): C-COLMN (CONTINUED)

NON-CONVENTIONAL COMPONENTS (KG/SEC)			
CCLOSE	0.000000E+00	0.000000E+00	0.000000E+00
ACLOSE	0.000000E+00	0.000000E+00	0.000000E+00
CLBOSE	0.000000E+00	0.000000E+00	0.000000E+00
GCOSE	8.60230	8.60230	0.000000E+00
ENZYME	0.000000E+00	0.000000E+00	0.000000E+00
HCLOSE	0.000000E+00	0.000000E+00	0.000000E+00
XYLOSE	9.99892	9.99892	0.000000E+00
LIGNIN	0.000000E+00	0.000000E+00	0.000000E+00
TOTAL BALANCE			
MASS (KG/SEC)	96.2539	96.2539	0.000000E+00
ENTHALPY (WATT)	-0.122307E+10	-0.122311E+10	0.353066E-04

*** INPUT DATA ***

FLASH SPECS FOR STREAM 16

TEMPERATURE (K)	MISSING
PRESSURE (N/SQM)	MISSING
VAPOR FRACTION	MISSING
PHASE CODE	2
TEMP ESTIMATE (K)	MISSING
PRES ESTIMATE (N/SQM)	MISSING
MAX. NO. ITERATIONS	25
CONVERGENCE TOL.	0.000100000

FLASH SPECS FOR STREAM 17

TEMPERATURE (K)	MISSING
PRESSURE (N/SQM)	MISSING
VAPOR FRACTION	MISSING
PHASE CODE	2
TEMP ESTIMATE (K)	MISSING
PRES ESTIMATE (N/SQM)	MISSING
MAX. NO. ITERATIONS	25
CONVERGENCE TOL.	0.000100000

FRACTION OF FEED

SUBSTREAM= MIXED			
STREAM= 16	CPT= H2SO4	FRACTION=	1.00000
	HMF		1.00000
	FURFURAL		1.00000

*** RESULTS ***

HEAT DUTY (WATT)	43.183.8
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SEPARATOR (SEP): C-COLUMN (CONTINUED)

COMPONENT = WATER		
STREAM	SUBSTREAM	SPLIT FRACTION
17	MIXED	1.00000

COMPONENT = H2SO4		
STREAM	SUBSTREAM	SPLIT FRACTION

COMPONENT = HMF		
STREAM	SUBSTREAM	SPLIT FRACTION
16	MIXED	1.00000

COMPONENT = FURFURAL		
STREAM	SUBSTREAM	SPLIT FRACTION
16	MIXED	1.00000

COMPONENT = CCLOSE		
STREAM	SUBSTREAM	SPLIT FRACTION

COMPONENT = ACLOSE		
STREAM	SUBSTREAM	SPLIT FRACTION

COMPONENT = CLBOSE		
STREAM	SUBSTREAM	SPLIT FRACTION

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SEPARATOR (SEP): C-COLMN (CONTINUED)

COMPONENT =	GCOSE	
STREAM	SUBSTREAM	SPLIT FRACTION
17	NCPSD	1.00000

COMPONENT =	ENZYME	
STREAM	SUBSTREAM	SPLIT FRACTION

COMPONENT =	HCLOSE	
STREAM	SUBSTREAM	SPLIT FRACTION

COMPONENT =	XYLOSE	
STREAM	SUBSTREAM	SPLIT FRACTION
17	NCPSD	1.00000

COMPONENT =	LIGNIN	
STREAM	SUBSTREAM	SPLIT FRACTION

DESCRIPTION OF STREAM CLASS MIXNCPSD

STREAM CLASS : MIXNCPSD
 SUBSTREAMS : MIXED NCPSD
 SUBSTRM CLASS: MIXED NCPSD
 SUBSTRM ATTR : PSD

DESCRIPTION OF STREAM CLASS HEAT

STREAM CLASS : HEAT
 STREAM ATTR : HEAT

DESCRIPTION OF STREAM CLASS WORK

STREAM CLASS : WORK
 STREAM ATTR : WORK

SUBSTREAM ATTR PSD TYPE: PSD

INTERVAL	LOWER LIMIT		UPPER LIMIT	
1	0.0	METER	.20000-03	METER
2	.20000-03	METER	.40000-03	METER
3	.40000-03	METER	.60000-03	METER
4	.60000-03	METER	.80000-03	METER
5	.80000-03	METER	0.0010	METER
6	0.0010	METER	0.0020	METER
7	0.0020	METER	0.0030	METER
8	0.0030	METER	0.0100	METER
9	0.0100	METER	0.0200	METER
10	0.0200	METER	0.0500	METER

2 3 6 7B 7C

STREAM ID	2	3	6	7B	7C
FROM :	CRUSHER	PUMP1	SLRYTNK	ACIDIN	HEATER1
TO :	PUMP1	SLRYTNK	ACIDIN	HEATER1	ACIDHYD
CLASS:	MIXNCPSD	MIXNCPSD	MIXNCPSD	MIXNCPSD	MIXNCPSD

SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL				
WATER	KG/SEC	45.4700	45.4700	84.4200	84.4200	84.4200
H2SO4	KG/SEC	0.0	0.0	0.0	1.9587	1.9587
HMF	KG/SEC	0.0	0.0	0.0	0.0	0.0
FURFURAL	KG/SEC	0.0	0.0	0.0	0.0	0.0
TOTAL	KG/SEC	45.4700	45.4700	84.4200	86.3787	86.3787
TEMP	K	300.1500	300.3159	468.2418	467.5981	468.1500
PRES	N/SQM	.10130+06	.14000+07	.14000+07	.14000+07	.14000+07
ENTHALPY	J/KG	-.15962+08	-.15960+08	-.14522+08	-.14210+08	-.12874+08
VFRAC		0.0	0.0	0.3233	0.3288	1.0000
LFRAC		1.0000	1.0000	0.6766	0.6711	0.0
ENTROPY	J/KG-K	-9267.7535	-9266.2742	-5803.1894	-5655.1047	-2799.5091
DENSITY	KG/CUM	846.6394	846.6829	21.0611	21.8864	7.0786
AVG MW		18.0150	18.0150	18.0150	18.3547	18.3547

SUBSTREAM: NCPSD		STRUCTURE: NON CONVENTIONAL				
CCLOSE	KG/SEC	19.6400	19.6400	19.6400	19.6400	19.6400
ACLOSE	KG/SEC	7.2400	7.2400	7.2400	7.2400	7.2400
CLBOSE	KG/SEC	0.0	0.0	0.0	0.0	0.0
GCOSE	KG/SEC	0.0	0.0	0.0	0.0	0.0
ENZYME	KG/SEC	0.0	0.0	0.0	0.0	0.0
HCLOSE	KG/SEC	10.7100	10.7100	10.7100	10.7100	10.7100
XYLOSE	KG/SEC	0.0	0.0	0.0	0.0	0.0
LIGNIN	KG/SEC	7.8800	7.8800	7.8800	7.8800	7.8800
TOTAL	KG/SEC	45.4700	45.4700	45.4700	45.4700	45.4700
TEMP	K	300.1500	300.3159	468.2418	467.5981	468.1500
PRES	N/SQM	.10130+06	.14000+07	.14000+07	.14000+07	.14000+07
ENTHALPY	J/KG	.69079+06	.69117+06	.10776+07	.10761+07	.10774+07
VFRAC		0.0	0.0	0.0	0.0	0.0
LFRAC		0.0	0.0	0.0	0.0	0.0
DENSITY	KG/CUM	705.4500	705.4500	705.4500	705.4500	705.4500
AVG MW		1.0000	1.0000	1.0000	1.0000	1.0000

COMPONENT ATTRIBUTES:
 ENZYME CAUSR1

	2	3	6	7B	7C
ELEM1	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM2	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM3	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM4	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM5	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM6	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM7	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM8	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM9	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM10	MISSING	MISSING	MISSING	MISSING	MISSING

SUBSTREAM ATTRIBUTES:
 PSD

2 3 6 7B 7C (CONTINUED)

STREAM ID	2	3	6	7B	7C
FRAC1	0.3289	0.3289	0.3289	0.3289	0.3289
FRAC2	0.1451	0.1451	0.1451	0.1451	0.1451
FRAC3	0.1266	0.1266	0.1266	0.1266	0.1266
FRAC4	0.1205	0.1205	0.1205	0.1205	0.1205
FRAC5	0.2542	0.2542	0.2542	0.2542	0.2542
FRAC6	0.0244	0.0244	0.0244	0.0244	0.0244
FRAC7	0.0	0.0	0.0	0.0	0.0
FRAC8	0.0	0.0	0.0	0.0	0.0
FRAC9	0.0	0.0	0.0	0.0	0.0
FRAC10	0.0	0.0	0.0	0.0	0.0

8 8A 8B 9 10

STREAM ID	8	8A	8B	9	10
FROM :	ACIDHYD	FICTSEP	FICTSEP	QUENCH	QUENCH
TO :	FICTSEP		QUENCH		COOLER
CLASS:	MIXNCPSD	MIXNCPSD	MIXNCPSD	MIXNCPSD	MIXNCPSD

SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL				
WATER	KG/SEC	82.9665	0.0	82.9665	5.2838	77.6826
H2SO4	KG/SEC	1.9587	1.9587	0.0	0.0	0.0
HMf	KG/SEC	1.1173	0.0	1.1173	1.0657	0.0515
FURFURAL	KG/SEC	0.7688	0.0	0.7688	0.7334	0.0354
TOTAL	KG/SEC	86.8114	1.9587	84.8527	7.0830	77.7696
TEMP	K	468.1500	468.1500	468.1500	373.1500	373.1500
PRES	N/SQM	.14000+07	.14000+07	.14000+07	.10130+06	.10130+06
ENTHALPY	J/KG	-.12627+08	-.89407+06	-.12898+08	-.10377+08	-.15616+08
VFRAC		1.0000	1.0000	1.0000	1.0000	0.0
LFRAC		0.0	0.0	0.0	0.0	1.0000
ENTROPY	J/KG-K	-2775.3276	8.5787-2852.2458	-2026.5210	-8274.1375	
DENSITY	KG/CUM	7.2163	35.9698	7.0860	0.7548	800.0021
AVG MW		18.7002	98.0800	18.3573	22.8932	18.0319

SUBSTREAM: NCPSD		STRUCTURE: NON CONVENTIONAL				
CCLOSE	KG/SEC	17.7014	0.0	17.7014	0.0	17.7014
ACLOSE	KG/SEC	0.0	0.0	0.0	0.0	0.0
CLBOSE	KG/SEC	0.0	0.0	0.0	0.0	0.0
GCLOSE	KG/SEC	8.6022	0.0	8.6022	0.0	8.6022
ENZYME	KG/SEC	0.0	0.0	0.0	0.0	0.0
HCLOSE	KG/SEC	0.8546	0.0	0.8546	0.0	0.8546
XYLOSE	KG/SEC	9.9989	0.0	9.9989	0.0	9.9989
LIGNIN	KG/SEC	7.8800	0.0	7.8800	0.0	7.8800
TOTAL	KG/SEC	45.0372	0.0	45.0372	0.0	45.0372
TEMP	K	468.1500	MISSING	468.1500	MISSING	373.1500
PRES	N/SQM	.14000+07	.14000+07	.14000+07	.10130+06	.10130+06
ENTHALPY	J/KG	.10774+07	MISSING	.10774+07	MISSING	.85878+06
VFRAC		0.0	MISSING	0.0	MISSING	0.0
LFRAC		0.0	MISSING	0.0	MISSING	0.0
DENSITY	KG/CUM	MISSING	MISSING	705.4500	MISSING	705.4500
AVG MW		1.0000	1.0000	1.0000	MISSING	1.0000

COMPONENT ATTRIBUTES:

ENZYME CAUSR1

	8	8A	8B	9	10
ELEM1	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM2	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM3	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM4	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM5	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM6	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM7	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM8	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM9	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM10	MISSING	MISSING	MISSING	MISSING	MISSING

SUBSTREAM ATTRIBUTES:
 PSD

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8 8A 8B 9 10 (CONTINUED)

STREAM ID	8	8A	8B	9	10
FRAC1	0.3289	0.3289	0.3289	0.3289	0.3289
FRAC2	0.1451	0.1451	0.1451	0.1451	0.1451
FRAC3	0.1266	0.1266	0.1266	0.1266	0.1266
FRAC4	0.1205	0.1205	0.1205	0.1205	0.1205
FRAC5	0.2542	0.2542	0.2542	0.2542	0.2542
FRAC6	0.0244	0.0244	0.0244	0.0244	0.0244
FRAC7	0.0	0.0	0.0	0.0	0.0
FRAC8	0.0	0.0	0.0	0.0	0.0
FRAC9	0.0	0.0	0.0	0.0	0.0
FRAC10	0.0	0.0	0.0	0.0	0.0

10A 11 12 13 14

STREAM ID	10A	11	12	13	14
FROM :	COOLER	CENFUG1	CENFUG1	CENFUG2	CENFUG2
TO :	CENFUG1	CENFUG3	CENFUG2	CENFUG3	
CLASS:	MIXNCPSD	MIXNCPSD	MIXNCPSD	MIXNCPSD	MIXNCPSD

SUBSTREAM: MIXED	STRUCTURE: CONVENTIONAL				
WATER KG/SEC	77.6826	77.5658	0.1168	0.0	0.1168
H2SO4 KG/SEC	0.0	0.0	0.0	0.0	0.0
HMF KG/SEC	0.0515	0.0514	.77467-04	0.0	.77467-04
FURFURAL KG/SEC	0.0354	0.0353	.53310-04	0.0	.53310-04
TOTAL KG/SEC	77.7696	77.6527	0.1169	0.0	0.1169
TEMP K	306.1500	306.1500	306.1500	MISSING	306.1500
PRES N/SQM	.10130+06	.10130+06	.10130+06	.10130+06	.10130+06
ENTHALPY J/KG	-.15919+08	-.15919+08	-.15919+08	MISSING	-.15919+08
VFRAC	0.0	0.0	0.0	MISSING	0.0
LFRAC	1.0000	1.0000	1.0000	MISSING	1.0000
ENTROPY J/KG-K	-9170.5223	-9170.5223	-9170.5223	MISSING	-9170.5223
DENSITY KG/CUM	843.4797	843.4797	843.4797	MISSING	843.4797
AVG MW	18.0319	18.0319	18.0319	MISSING	18.0319

SUBSTREAM: NCPSD	STRUCTURE: NON CONVENTIONAL				
CCLOSE KG/SEC	17.7014	0.0	17.7014	0.0	17.7014
ACLOSE KG/SEC	0.0	0.0	0.0	0.0	0.0
CLBOSE KG/SEC	0.0	0.0	0.0	0.0	0.0
GCOSE KG/SEC	8.6022	0.0	8.6022	8.6022	0.0
ENZYME KG/SEC	0.0	0.0	0.0	0.0	0.0
HCLOSE KG/SEC	0.8546	0.0	0.8546	0.0	0.8546
XYLOSE KG/SEC	9.9989	0.0	9.9989	9.9989	0.0
LIGNIN KG/SEC	7.8800	0.0	7.8800	0.0	7.8800
TOTAL KG/SEC	45.0372	0.0	45.0372	18.6012	26.4360
TEMP K	306.1500	MISSING	306.1500	306.1500	306.1500
PRES N/SQM	.10130+06	.10130+06	.10130+06	.10130+06	.10130+06
ENTHALPY J/KG	.70460+06	MISSING	.70460+06	.70460+06	.70460+06
VFRAC	0.0	MISSING	0.0	0.0	0.0
LFRAC	0.0	MISSING	0.0	0.0	0.0
DENSITY KG/CUM	705.4500	MISSING	705.4500	705.4500	705.4500
AVG MW	1.0000	1.0000	1.0000	1.0000	1.0000

COMPONENT ATTRIBUTES:
 ENZYME CAUSR1

ELEM1	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM2	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM3	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM4	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM5	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM6	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM7	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM8	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM9	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM10	MISSING	MISSING	MISSING	MISSING	MISSING

SUBSTREAM ATTRIBUTES:
 PSD

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10A 11 12 13 14 (CONTINUED)

STREAM ID	10A	11	12	13	14
FRAC1	0.3289	MISSING	0.3289	0.3289	0.3289
FRAC2	0.1451	MISSING	0.1451	0.1451	0.1451
FRAC3	0.1266	MISSING	0.1266	0.1266	0.1266
FRAC4	0.1205	MISSING	0.1205	0.1205	0.1205
FRAC5	0.2542	MISSING	0.2542	0.2542	0.2542
FRAC6	0.0244	MISSING	0.0244	0.0244	0.0244
FRAC7	0.0	MISSING	0.0	0.0	0.0
FRAC8	0.0	MISSING	0.0	0.0	0.0
FRAC9	0.0	MISSING	0.0	0.0	0.0
FRAC10	0.0	MISSING	0.0	0.0	0.0

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15 16 17 1 4

STREAM ID	15	16	17	1	4
FROM :	CENFUG3	C-COLUMN	C-COLUMN		
TO :	C-COLUMN			CRUSHER	SLRYTNK
CLASS:	MIXNCPSD	MIXNCPSD	MIXNCPSD	MIXNCPSD	MIXNCPSD

SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL				
WATER	KG/SEC	77.5658	0.0	77.5658	45.4700	38.9500
H2SO4	KG/SEC	0.0	0.0	0.0	0.0	0.0
HMF	KG/SEC	0.0514	0.0514	0.0	0.0	0.0
FURFURAL	KG/SEC	0.0353	0.0353	0.0	0.0	0.0
TOTAL	KG/SEC	77.6527	0.0868	77.5658	45.4700	38.9500
TEMP	K	306.1500	306.1500	306.1500	300.1500	826.9415
PRES	N/SQM	.10130+06	.10130+06	.10130+06	.10130+06	.14000+07
ENTHALPY	J/KG	-.15919+08	-.23134+07	-.15935+08	-.15962+08	-.12391+08
VFRAC		0.0	0.0	0.0	0.0	1.0000
LFRAC		1.0000	1.0000	1.0000	1.0000	0.0
ENTROPY	J/KG-K	-9170.5223	-3490.7728	-9178.5314	-9267.7535	-1674.5832
DENSITY	KG/CUM	843.4797	1162.9854	843.2512	846.6394	3.7048
AVG MW		18.0319	111.8070	18.0150	18.0150	18.0150

SUBSTREAM: NCPSD		STRUCTURE: NON CONVENTIONAL				
CCLOSE	KG/SEC	0.0	0.0	0.0	19.6400	0.0
ACLOSE	KG/SEC	0.0	0.0	0.0	7.2400	0.0
CLBOSE	KG/SEC	0.0	0.0	0.0	0.0	0.0
GCOSE	KG/SEC	8.6022	0.0	8.6022	0.0	0.0
ENZYME	KG/SEC	0.0	0.0	0.0	0.0	0.0
HCLOSE	KG/SEC	0.0	0.0	0.0	10.7100	0.0
XYLOSE	KG/SEC	9.9989	0.0	9.9989	0.0	0.0
LIGNIN	KG/SEC	0.0	0.0	0.0	7.8800	0.0
TOTAL	KG/SEC	18.6012	0.0	18.6012	45.4700	0.0
TEMP	K	306.1500	MISSING	306.1500	300.1500	MISSING
PRES	N/SQM	.10130+06	.10130+06	.10130+06	.10130+06	MISSING
ENTHALPY	J/KG	.70460+06	MISSING	.70460+06	.69079+06	MISSING
VFRAC		0.0	MISSING	0.0	0.0	MISSING
LFRAC		0.0	MISSING	0.0	0.0	MISSING
DENSITY	KG/CUM	705.4500	MISSING	705.4500	705.4500	MISSING
AVG MW		1.0000	1.0000	1.0000	1.0000	1.0000

COMPONENT ATTRIBUTES:

ENZYME CAUSR1

	15	16	17	1	4
ELEM1	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM2	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM3	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM4	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM5	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM6	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM7	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM8	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM9	MISSING	MISSING	MISSING	MISSING	MISSING
ELEM10	MISSING	MISSING	MISSING	MISSING	MISSING

SUBSTREAM ATTRIBUTES:

PSD

15 16 17 1 4 (CONTINUED)

STREAM ID	15	16	17	1	4
FRAC1	0.3289	0.3289	0.3289	0.0	MISSING
FRAC2	0.1451	0.1451	0.1451	0.0	MISSING
FRAC3	0.1266	0.1266	0.1266	0.0	MISSING
FRAC4	0.1205	0.1205	0.1205	0.0	MISSING
FRAC5	0.2542	0.2542	0.2542	0.0	MISSING
FRAC6	0.0244	0.0244	0.0244	0.0	MISSING
FRAC7	0.0	0.0	0.0	0.0	MISSING
FRAC8	0.0	0.0	0.0	0.0	MISSING
FRAC9	0.0	0.0	0.0	0.5000	MISSING
FRAC10	0.0	0.0	0.0	0.5000	MISSING

7

STREAM ID 7
 FROM :
 TO : ACIDIN
 CLASS: MIXNCPSD

SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL
WATER	KG/SEC	0.0
H2SO4	KG/SEC	1.9587
HMF	KG/SEC	0.0
FURFURAL	KG/SEC	0.0
TOTAL	KG/SEC	1.9587
TEMP	K	759.3750
PRES	N/SQM	.14000+07
ENTHALPY	J/KG	-.80399+06
VFRAC		1.0000
LFRAC		0.0
ENTROPY	J/KG-K	158.1272
DENSITY	KG/CUM	21.7546
AVG MW		98.0800

SUBSTREAM: NCPSD		STRUCTURE: NON CONVENTIONAL
CCLOSE	KG/SEC	0.0
ACLOSE	KG/SEC	0.0
CLBOSE	KG/SEC	0.0
GCOSE	KG/SEC	0.0
ENZYME	KG/SEC	0.0
HCLOSE	KG/SEC	0.0
XYLOSE	KG/SEC	0.0
LIGNIN	KG/SEC	0.0
TOTAL	KG/SEC	0.0
TEMP	K	MISSING
PRES	N/SQM	MISSING
ENTHALPY	J/KG	MISSING
VFRAC		MISSING
LFRAC		MISSING
AVG MW		1.0000
COMPONENT ATTRIBUTES:		
ENZYME	CAUSR1	
ELEM1		MISSING
ELEM2		MISSING
ELEM3		MISSING
ELEM4		MISSING
ELEM5		MISSING
ELEM6		MISSING
ELEM7		MISSING
ELEM8		MISSING
ELEM9		MISSING
ELEM10		MISSING
SUBSTREAM ATTRIBUTES:		
PSD		
FRAC1		MISSING

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QHTR QACHYD QQNCH QCOOLR

STREAM ID	QHTR	QACHYD	QQNCH	QCOOLR
FROM :	HEATER1	ACIDHYD	QUENCH	COOLER
TO :				
CLASS:	HEAT	HEAT	HEAT	HEAT

STREAM ATTRIBUTES:

HEAT				
Q	WATT	-.11547+09-	.15400+08	.20338+09 .30551+08

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SHAFT1

STREAM ID	SHAFT1
FROM :	PUMP1
TO :	
CLASS:	WORK

STREAM ATTRIBUTES:

WORK	
P	WATT. .10731+06